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(54) Title: PROTEIN CRYSTAL STRUCTURE AND METHOD FOR IDENTIFYING PROTEIN MODULATORS

(57) Abstract: A method of identifying an agent compound (such as an inhibitor) which modulates asparate decarboxylase (ADC) activity. The method comprises the steps of: a) providing a model of a binding cavity of ADC, said model including at least one of binding site nos. 1 and 9 defined by Table 2; b) providing the structure of said agent compound; c) fitting the candidate agent compound to said binding cavity, including determining the interactions between the candidate agent compound and at least one of binding site nos. 1 and 9; and d) selecting the candidate agent compound.

PROTEIN CRYSTAL STRUCTURE AND METHOD FOR IDENTIFYING PROTEIN MODULATORS

Field of the Invention

The present invention relates to the enzyme aspartate decarboxylase, and in particular the use of its crystal structure for drug discovery.

Background of the Invention

Pantothenic acid (vitamin B_5) is found in coenzyme A (CoA) and the acyl carrier protein (ACP), both of which are involved in fatty acid metabolism.

Pantothenic acid can be synthesised by plants and microorganisms but animals are apparently unable to make the vitamin, and require it in their diet. However, all organisms are able to convert pantothenic acid to its metabolically active form, coenzyme A.

The pathway for the synthesis of pantothenic acid in bacteria is shown in Fig. 1. It provides a potential target for the treatment of infectious disease, since inhibitors of the pathway should be damaging to microorganisms but not to human or animal subjects infected by microorganisms.

Of specific interest is aspartate decarboxylase (L-aspartate-α-decarboxylase (EC 4.1.1.1)). This enzyme catalyses the decarboxylation of L-aspartate to β-alanine, which then goes on to form pantothenate in a condensation reaction with D-pantoate. Inhibitors (whether competitive, non-competitive, uncompetitive or irreversible) of aspartate decarboxylase (ADC) would be of significant technical and commercial interest.

ADC was first isolated from *Escherichia coli* by Williamson *et al.* (*J. Biol. Chem.*, 254, (1979), 8074-8082), who found indications that the protein was present in

different processed states. The unprocessed enzyme is referred to as the π-chain and has 126 residues. Processing (see Fig. 2) splits the π-chain at the Gly24-Ser25 peptide bond into a larger C-terminal chain and a smaller N-terminal chain. A pyruvol group (for convenience termed Pvl25) is generated from the serine residue (Ser25) at the end of the C-chain, and a carboxylate group is formed at the end of the glycine residue (Gly24) of the smaller N-terminal chain. Williamson *et al.* found that only a proportion of the enzyme chains were processed in this way.

Purification to homogeneity of overexpressed, recombinant ADC was achieved by Ramjee *et al.* (*J. Biochem.*, 323, (1997), 661-669). The purified enzyme was found to be a tetramer which, after processing, contained three processed chains and one chain which was not fully processed.

Albert *et al.* (*Nature Structural Biology*, 5, (1998), 289-293) used X-ray crystallography to determine the structure of ADC to 2.2 Å resolution. They showed that the enzyme studied by Ramjee *et al.* has pseudo-fourfold rotational symmetry, each of the four tetramer subunits (each subunit or corresponding to a π-chain labelled A, B, C or D) having a six-stranded β-barrel capped by small α-helices at each end. The binding cavities for aspartate decarboxylation are located between adjacent subunits. Three of the binding cavities have catalytic pyruvol groups resulting from respective processed π-chains. The other binding cavity has an ester which appears to be an intermediate in the processing reaction. The evidence points to an autocatalytic self-processing mechanism which did not lead to full processing of all the π-chains. The coordinates of the crystal structure determined by Albert *et al.* are available from the Protein Data Bank (Berman *et al.*, *Nucleic Acids Research*, 28, (2000), 235-242) under access code 1AW8.

Albert *et al.* proposed a model of L-asparate binding, but did not suggest a mechanism by which ADC accomplishes aspartate decarboxylation. Until now very little was known about the enzyme's role in catalysis. This has impeded the development of ADC inhibitors via structure-based drug design methodologies. Knowledge of the mechanism would significantly assist the rational design of novel therapeutics based on ADC inhibitors.

Definitions

Specific residues are denoted herein by their conventional acronyms (e.g. Gly for glycine), and numbers corresponding to their position in the unprocessed π-chain counting from the N-terminal of the π-chain (e.g. Gly24). Moreover, because each binding cavity is formed from the residues of two π-chains, each residue is further denoted by a letter corresponding to the respective one of the π-chains (e.g. Gly24A or Lys9D). Below, we have used D and A to denote the two π-chains of a binding cavity, but in a tetramer with four equivalent binding cavities and subunits labelled A, B, C and D one could equally use A and B, B and C, or C and D instead.

In the following by "binding site" we mean a site, such as an atom or functional group of an amino acid residue, in the ADC binding cavity which may bind to an agent compound such as a candidate inhibitor. Depending on the particular molecule in the cavity, sites may exhibit attractive or repulsive binding interactions, brought about by charge, steric considerations and the like.

By "fitting", is meant determining by automatic, or semi-automatic means, interactions between one or more atoms of an agent molecule and one or more atoms or binding sites of the ADC, and determining the extent to which such interactions are

stable. Various computer-based methods for fitting are described further herein.

By "fully processed" ADC we mean a composition comprising an amount of ADC in which pyruvoyl groups are generated from at least 90%, preferably at least 95%, and more preferably at least 99% of the ADC Ser25 residues.

By "root mean square deviation" we mean the square root of the arithmetic mean of the squares of the deviations from the mean.

By a "computer system" we mean the hardware means, software means and data storage means used to analyse atomic coordinate data. The minimum hardware means of the computer-based systems of the present invention typically comprises a central processing unit (CPU), input means, output means and data storage means. Desirably a monitor is provided to visualise structure data. The data storage means may be RAM or means for accessing computer readable media of the invention. Examples of such systems are microcomputer workstations available from Silicon Graphics Incorporated and Sun Microsystems running Unix based, Windows NT or IBM OS/2 operating systems.

By "computer readable media" we mean any media which can be read and accessed directly by a computer e.g. so that the media is suitable for use in the above-mentioned computer system. The media include, but are not limited to: magnetic storage media such as floppy discs, hard disc storage medium and magnetic tape; optical storage media such as optical discs or CD-ROM; electrical storage media such as RAM and ROM; and hybrids of these categories such as magnetic/optical storage media.

Summary of the Invention

The present invention is at least partly based on overcoming several technical hurdles: we have (i) produced fully processed ADC, (ii) produced crystals of ADC of suitable quality for performing X-ray diffraction analyses (in particular we have produced crystals which diffract X-rays for the determination of atomic coordinates of ADC to a resolution which is better, i.e. numerically lower, than 2 Å), (iii) formed ADC-ligand complexes by soaking the crystals in appropriate soaking solutions, (iv) collected X-ray diffraction data from the ADC-ligand complexes, (v) determined the three-dimensional structures of the complexes, (vi) identified regions of ADC which undergo conformational changes upon ligand binding and decarboxylation, and (vii) determined the likely mechanism by which ADC accomplishes aspartate decarboxylation.

In general aspects, the present invention is concerned with identifying or obtaining agent compounds (especially inhibitors of ADC) for modulating ADC activity, and in preferred embodiments identifying or obtaining actual agent compounds/inhibitors. Crystal structure information presented herein is useful in designing potential inhibitors and modelling them or their potential interaction with the ADC binding cavity. Potential inhibitors may be brought into contact with ADC to test for ability to interact with the ADC binding cavity. Actual inhibitors may be identified from among potential inhibitors synthesized following design and model work performed *in silico*. An inhibitor identified using the present invention may be formulated into a composition, for instance a composition comprising a pharmaceutically acceptable excipient, and may be used in the manufacture of a medicament for use in a method of treatment. These and other

aspects and embodiments of the present invention are discussed below.

A first aspect of the invention provides a crystal of fully processed ADC. The crystal may have unit cell dimensions of a = 71.1 Å ± 5%, and c = 215.8 Å ± 5%. Preferably, a = 71.1 Å, and c = 215.8 Å, or more generally a = 71.1±0.2 Å, and c = 215.8±0.2 Å. Preferably the crystal of fully processed ADC has the hexagonal point group 622, and more preferably the space group $P6_122$.

A further aspect of the invention provides a crystal of (preferably fully processed) ADC which diffract X-rays for the determination of atomic coordinates of ADC to a resolution which is better than 2 Å.

Alternatively or additionally, the crystal has the three dimensional atomic coordinates of Table 1. An advantageous feature of the structural data according to Table 1 are that they have a high resolution of about 1.55 Å.

The coordinates of Table 1 provide a measure of atomic location in Angstroms, to a first decimal place. The coordinates are a relative set of positions that define a shape in three dimensions. It is possible that an entirely different set of coordinates having a different origin and/or axes could define a similar or identical shape. Furthermore, varying the relative atomic positions of the atoms of the structure so that the root mean square deviation of the conserved residue backbone atoms (i.e. the nitrogen-carbon-carbon backbone atoms of the protein amino acid residues) is less than 1.5 Å (preferably less than 1.0 Å and more preferably less than 0.5 Å) when superimposed on the coordinates provided in Table 1 for the conserved residue backbone atoms, will generally result in a structure which is substantially the same as the structure of Table 1 in terms of both its structural characteristics and potency for structure-

based drug design of ADC inhibitors. Likewise changing the number and/or positions of the water molecules of Table 1 will not generally affect the potency of the structure for structure-based drug design of ADC inhibitors. Thus for the purposes described herein as being aspects of the present invention, it is within the scope of the invention if: the Table 1 coordinates are transposed to a different origin and/or axes; the relative atomic positions of the atoms of the structure are varied so that the root mean square deviation of conserved residue backbone atoms is less than 1.5 Å (preferably less than 1.0 Å and more preferably less than 0.5 Å) when superimposed on the coordinates provided in Table 1 for the conserved residue backbone atoms; and/or the number and/or positions of water molecules is varied. Reference herein to the coordinates of Table 1 thus includes the coordinates in which one or more individual values of the Table are varied in this way.

Also, modifications in the ADC crystal structure due to e.g. mutations, additions, substitutions, and/or deletions of amino acid residues (including the deletion of one or more tetramer subunits) could account for variations in the ADC atomic coordinates. However, atomic coordinate data of ADC modified so that a ligand that bound to one or more binding sites of ADC would also be expected to bind to the corresponding binding sites of the modified ADC are, for the purposes described herein as being aspects of the present invention, also within the scope of the invention. Reference herein to the coordinates of Table 1 thus includes the coordinates modified in this way. Preferably, the modified coordinate data define at least one ADC binding cavity.

We have been able to produce and isolate for the first time fully-processed ADC, in which the binding cavities of substantially all the ADC molecules are identical and each

binding cavity has a catalytic pyruvol group. This has been made possible by the identification of conditions which allow the processing reaction to proceed to completion.

The present invention contemplates also "mutants", wherein by a "mutant" we mean a polypeptide which is obtained by replacing at least one amino acid residue in ADC with a different amino acid residue and/or by adding and/or deleting amino acid residues within ADC or at the N- and/or C-terminus of ADC and which has substantially the same three-dimensional structure as ADC from which it is derived. By having substantially the same three-dimensional structure is meant having a set of atomic structure co-ordinates that have a root mean square deviation of less than or equal to about 2.0 Å when superimposed with the atomic structure co-ordinates of the ADC from which the mutant is derived when at least about 50% to 100% of the C_α atoms of the ADC are included in the superposition.

To produce mutants, amino acids present in ADC can be replaced by other amino acids having similar properties, for example hydrophobicity, hydrophobic moment, propensity to form or break α-helical or β-sheet structures, and so on. Substitutional variants of a protein are those in which at least one amino acid in the protein sequence has been removed and a different residue inserted in its place. Amino acid substitutions are typically of single residues but may be clustered depending on functional constraints e.g. at a crystal contact. Preferably amino acid substitutions will comprise conservative amino acid substitutions. Insertional amino acid variants are those in which one or more amino acids are introduced. This can be amino-terminal and/or carboxy-terminal fusion as well as intrasequence.

Thus the previous aspects of the invention relating to crystals of ADC, may be extended to crystals of mutant ADC.

A further aspect of the invention provides a method of fully processing ADC comprising the step of forming a solution of ADC, the solution having a pH in the range 6.5-8.5 (preferably 7.0-8.0) and an ADC concentration in the range 1-50 mg/ml (preferably 4-20 mg/ml).

The method may further comprise the step of crystallising the dissolved ADC to form a crystal of fully processed ADC.

In a further aspect, the invention provides a method for growing a crystal of (preferably fully processed) ADC, which method comprises: forming a 1:1 mixture of a crystallising solution containing 1.6 to 2.4 M $Na_2(SO_4)$ and a protein solution containing ADC at a concentration of 6 to 10 mg/ml in 25 mM HEPES buffer at pH 7.5; and growing the crystal by vapour diffusion from the mixture.

In a further aspect, the invention provides a method of testing a candidate agent compound (such as a candidate inhibitor of ADC) for ability to modulate ADC activity comprising the step of contacting the candidate agent compound with fully processed ADC (produced e.g. according to the method of the one of the previous aspects) to determine the ability of the candidate agent compound to interact with ADC.

Preferably, the candidate agent compound is contacted with ADC in the presence of L-aspartate, and typically a buffer.

By using fully processed ADC for forming ADC-ligand complexes more candidate agent compound molecules per molecule of ADC are exposed to fully processed binding cavities, thereby increasing the sensitivity of e.g. chemical assays based on such complexes.

The above aspects of the invention, both singly and in combination, all contribute to features of the invention which are advantageous.

The structure of fully processed ADC can also be used to solve the crystal structure of proteins, such as ADC-ligand complexes or ADC chimaera-ligand complexes (ADC chimaeras are discussed below) of unknown structure, where X-ray diffraction data or NMR spectroscopic data of these targets has been generated and requires interpretation in order to provide the structure.

Thus, where X-ray crystallographic or NMR spectroscopic data is provided for a target ADC-ligand complex, or an ADC chimaera-ligand complex of unknown three-dimensional structure, the structure of fully processed ADC as defined by Table 1 may be used to interpret that data to provide a likely structure for the target by techniques which are well known in the art, e.g. phasing in the case of X-ray crystallography and assisting peak assignments in NMR spectra.

One method that may be employed for these purposes is molecular replacement. This method can provide an accurate structural form for the unknown structure more quickly and efficiently than attempting to determine such information *ab initio*. Examples of computer programs known in the art for performing molecular replacement are CNX (Brunger et al., *Current Opinion in Structural Biology*, 8, Issue 5, October 1998, 606-611, and commercially available from Accelerys, San Diego, CA) and AMORE (Navaza, *Acta Crystallographica*, A50, (1994), 157-163).

Thus, a further aspect of the invention provides a method for determining the structure of a protein, which method comprises;

providing the co-ordinates of Table 1; and

either (a) positioning the co-ordinates in the crystal unit cell of said protein so as to provide a structure for said protein, or (b) assigning NMR spectra peaks of said protein by manipulating the co-ordinates of Table 1.

In a further aspect the invention provides a method for determining the structure of a compound bound to ADC, said method comprising:

providing a crystal of ADC;

soaking the crystal with the compound to form a complex; and

determining the structure of the complex by employing the data of Table 1.

Alternatively, the ADC and the compound may be co-crystallized. Thus the invention provides a method for determining the structure of a compound bound to ADC, said method comprising:

mixing ADC with the compound;

crystallizing a ADC-compound complex; and

determining the structure of the complex by employing the data of Table 1.

A mixture of compounds may be soaked or co-crystallized with the crystal, wherein only one or some of the compounds may be expected to bind to the ADC. As well as the structure of the complex, the identity of the complexing compound(s) is/are then determined.

In a further aspect, the invention provides a method for determining the structure of a modulator of ADC bound to fully processed ADC, said method comprising:

providing a crystal of fully processed ADC according to the invention;

soaking the crystal with said modulator; and

determining the structure of said ADC-modulator complex.

Alternatively, the ADC and modulator may be co-crystallized. In either case, L-aspartate, β-alanine or an analogue thereof may optionally be present.

In a further aspect, the invention provides a method of analysing an ADC-ligand complex comprising the step of

employing (i) X-ray crystallographic diffraction data from the ADC-ligand complex and (ii) a three-dimensional structure of fully processed ADC, to generate a difference Fourier electron density map of the complex, the three-dimensional structure being defined by atomic coordinate data according to Table 1.

Preferably, the ADC is itself fully processed in the ADC-ligand complexes of the previous aspects.

Therefore, such complexes can be crystallised and analysed using X-ray diffraction methods, e.g. according to the approach described by Greer *et al.*, *J. of Medicinal Chemistry*, Vol. 37, (1994), 1035-1054, and difference Fourier electron density maps can be calculated based on X-ray diffraction patterns of soaked or co-crystallised ADC and the solved structure of fully processed un-complexed ADC. These maps can then be used to determine whether and where a particular ligand binds to ADC and/or changes the conformation of ADC.

Electron density maps can be calculated using programs such as those from the CCP4 computing package (Collaborative Computational Project 4. The CCP4 Suite: Programs for Protein Crystallography, *Acta Crystallographica*, D50, (1994), 760-763.). For map visualisation and model building programs such as *O* (Jones et al., *Acta Crystallograhy*, A47, (1991), 110-119) can be used.

In a further aspect, the invention provides a method of identifying an agent compound (such as an inhibitor of ADC) which modulates ADC activity comprising the steps of:

a) providing a candidate agent compound;

b) forming a complex of fully processed ADC (produced e.g. according to the method of one of the previous aspects) and the candidate agent compound; and

c) analysing said complex by X-ray crystallography (e.g. according to the method of one of the previous aspects) or by

NMR spectroscopy to determine the ability of said candidate agent compound to interact with ADC. Detailed structural information can then be obtained about the binding of the agent compound to ADC, and in the light of this information adjustments can be made to the structure or functionality of the agent compound, e.g. to improve binding to the binding cavity. Steps b) and c) may be repeated and re-repeated as necessary. For X-ray crystallographic analysis, the complex may be formed by crystal soaking or co-crystallisation.

Therefore, compared to partially processed ADC, X-ray crystallographic data from the binding cavities of fully processed ADC-ligand complexes can be interpreted more easily because all the binding cavities are identical. That is, the data are not complicated by reflections from binding sites containing esters instead of pyruvol groups. Likewise the interpretation of NMR spectra is simplified.

In a further aspect, the present invention provides a method of identifying an agent compound (such as an inhibitor of ADC) which modulates ADC activity, comprising the steps of:

a) providing a model of a binding cavity of ADC, said model including at least one (and preferably both) of binding site nos. 1 and 9 defined by Table 2;

b) providing the structure of a candidate agent compound;

c) fitting the candidate agent compound to said binding cavity, including determining the interactions between the candidate agent compound and at least one (and preferably both) of binding site nos. 1 and 9; and

d) selecting the fitted candidate agent compound.

Without wishing to be held to any particular theory, we believe that, in the appropriate context (e.g. in the complexes described below in the "Detailed Description of the Invention"), one or more of the binding sites of Table 2 provides the corresponding binding interaction of Table 2 to

an agent compound. However, the binding interactions of Table 2 are not intended to be exhaustive, and it is within the scope of this aspect of the invention that any of the binding sites may exhibit an interaction which is not listed in Table 2.

Varying the relative positions of the binding sites of Table 2 by relatively small amounts generally results in arrangements of binding sites which are substantially identical to the arrangement of Table 2 in terms of expected interactions with the agent compound. Consequently, the scope of this aspect of the invention includes a binding cavity in which the root mean square deviation of the conserved residue backbone atoms of the residues of column 2 of Table 2 is less than 1.5 Å (preferably less than 1.0 Å and more preferably less than 0.5 Å) when superimposed on the coordinates provided in Table 1 for the conserved residue backbone atoms of the residues of column 2 of Table 2.

The smaller N-terminal β-chain has a tail (hereafter called Tail24A) formed when the π-chain cleaves at the Gly24-Ser25 peptide bond and consisting of the four residues His21A, Tyr22A, Glu23A, and Gly24A (as discussed above, Gly24A having a carboxylate end group). We have found that Tail24A shifts between an "open" and a "closed" position via a "half-closed" position (which we call the O-state, C-state and H-state respectively) during aspartate decarboxylation. In the C-state Tail24A obstructs the binding cavity, while the O-state allows access thereto. These states are characterised by increased disorder in the measured position of Tail24A as it shifts from the C-state to the O-state.

Binding site no. 1 is associated with the hydrophobic phenyl ring of Tyr22A which in turn belongs to Tail24A. Hence binding site no. 1 is closely involved with the C-, H- and O-states of Tail24A.

The NH_3^+ group (binding site no. 9) of the Lys9D side chain is a potential hydrogen bond donor when Tail24A is in the O- and H-states. However, we have found that in the C-state the Gly24A carboxylate end group forms a salt bridge or hydrogen bond with the NH_3^+ group of the Lys9D side chain. This prevents the NH_3^+ group from being a potential hydrogen bond donor to the agent compound in the C-state.

The modelling may include generating the cavity (and optionally the agent compound) on a computer screen for visual inspection.

In practice, it is desirable to model a sufficient number of atoms of the ADC as defined by the coordinates of Table 1. Thus, in this aspect of the invention, there will preferably be provided the coordinates of at least 5, preferably at least 10, more preferably at least 50 and even more preferably at least 100 atoms of the ADC structure.

Preferred candidate agent compounds bind with at least two, three, four, five, six or seven of the binding sites defined by Table 2. In general, the agent compound binds better as the strength and number of binding interactions increases. The candidate agent compound may have a molecular weight of up to about 600.

Binding interactions may be mediated by e.g. water or other solvent molecules.

Candidate inhibitors identified according to the method are characterised by their suitability for binding to a particular binding site or sites. The binding cavity can therefore be regarded as a type of binding site framework or negative template with which the candidate inhibitors correlate in the manner described above.

Modulators of ADC may be inhibitors of the enzyme or compounds which affect its specificity or activity in relation to L-aspartate in other ways. The invention is particularly

suitable for the design, screening and development of ADC inhibitor components. It is thus a preferred aspect of the invention that modulating agent compounds are inhibitors.

The step of providing the structure of a candidate modulator molecule may involve selecting the compound by computationally screening a database of compounds for interaction with the binding cavity or cavities. For example, a 3-D descriptor for the potential modulator may be derived, the descriptor including geometric and functional constraints derived from the architecture and chemical nature of the binding cavity or cavities. The descriptor may then be used to interrogate the compound database, a potential modulator being a compound that has a good match to the features of the descriptor. In effect, the descriptor is a type of virtual pharmacophore.

In any event, the identification of ADC binding sites and interactions provides a basis for the design of new and specific ligands for ADC. For example, knowing the binding sites of ADC, computer modelling programs may be used to design different molecules expected to interact with possible or confirmed binding cavities or other structural or functional features of ADC.

More specifically, a potential modulator of ADC activity can be examined through the use of computer modelling using a docking program such as GRAM, DOCK, or AUTODOCK (see Walters *et al., Drug Discovery Today,* Vol.3, No.4, (1998), 160-178, and Dunbrack *et al., Folding and Design,* 2, (1997), 27-42) to identify candidate inhibitors of ADC. This procedure can include computer fitting of candidate inhibitors to ADC to ascertain how well the shape and the chemical structure of the candidate inhibitor will bind to the enzyme.

Computer programs can be employed to estimate the interactions between the ADC and the agent compound. The more

specificity in the design of a candidate drug, the more likely it is that the drug will not interact with other proteins as well. This will tend to minimise side-effects due to unwanted interactions with other proteins.

In one embodiment a plurality of candidate agent compounds are screened or interrogated for interaction with the binding sites. In one example, step (b) involves providing the structures of the candidate agent compounds, each of which is then fitted in step (c) to computationally screen a database of compounds (such as the Cambridge Structural Database) for interaction with the binding sites, i.e. the candidate agent compound is selected by computationally screening a database of compounds for interaction with the binding cavity. In another example, a 3-D descriptor for the agent compound is derived, the descriptor including e.g. geometric and functional constraints derived from the architecture and chemical nature of the binding cavity or cavities. The descriptor may then be used to interrogate the compound database, the identified agent compound being the compound which matches with the features of the descriptor. For example, the model resulting from step a) may be used to interrogate the compound database, a candidate inhibitor being a compound that has a good match to the features of the model. In effect, the descriptor is a type of virtual pharmacophore.

If one or more additional ADC binding cavities are characterised and a plurality of respective compounds are designed or selected, the candidate inhibitor may be formed by linking the respective compounds into a larger compound which maintains the relative positions and orientations of the respective compounds at the binding cavities. The larger compound may be formed as a real molecule or by computer modelling.

Thus the indentification of the ADC binding sites allows the development of compounds which interact with the binding cavity regions of ADC (for example to act as inhibitors of ADC) based on a fragment linking or fragment growing approach. For example, the binding of one or more molecular fragments can be determined in the protein binding cavity by X-ray crystallography. Molecular fragments are typically compounds with a molecular weight between 100 and 200 Da. This can then provide a starting point for medicinal chemistry to optimize the interactions using a structure-based approach. The fragments can be combined onto a template or used as the starting point for 'growing out' an inhibitor into other cavities of the protein. The fragments can be positioned in the binding cavity or cavities of ADC and then 'grown' to fill the space available, exploring the electrostatic, van der Waals or hydrogen-bonding interactions that are involved in molecular recognition. The potency of the original weakly binding fragment thus can be rapidly improved using iterative structure-based chemical synthesis.

At one or more stages in the fragment growing approach, the compound may be synthesized and tested in a biological system for its activity. This can be used to guide the further growing out of the fragment.

Where two fragment-binding regions are identified, a linked fragment approach may be based upon attempting to link the two fragments directly, or growing one or both fragments in the manner described above in order to obtain a larger, linked structure which may have the desired properties.

Having determined possible binding partners, these can then be obtained or synthesised and screened for activity. Consequently, the method preferably comprises the further step of:

e) contacting the candidate agent compound with ADC to determine the ability of the candidate agent compound to interact with ADC.

Preferably, in step e) the candidate agent compound is contacted with ADC in the presence of L-aspartate, and typically a buffer.

Instead of, or in addition to, performing a chemical assay, the method may comprise the further steps of:

e) forming a complex of ADC and said candidate agent compound; and

f) analysing said complex by X-ray crystallography (e.g. according to the method of the previous aspects of the invention) or by NMR spectroscopy to determine the ability of said candidate agent compound to interact with ADC.

Detailed structural information can then be obtained about the binding of the candidate agent compound to ADC, and in the light of this information adjustments can be made to the structure or functionality of the candidate agent compound, e.g. to improve binding to the binding cavity. Steps e) and f) may then be repeated and re-repeated as necessary. For X-ray crystallographic analysis, the complex may be formed by crystal soaking or co-crystallisation.

In a further general aspect, the invention relates to chimaeric proteins which have the binding specificities of ADC.

The use of chimaeric proteins to achieve desired properties is now common in the scientific literature. For example, Sieber et al. (*Nature Biotechnology*, 19, (2001), 456-460) produced hybrids between human cytochrome P450 isoform 1A2 and the bacterial P450 BM3, in order to make proteins with the specificity of 1A2, but which had desirable expression and solubility properties of BM3. Active site chimaeras are also described for example by Swairjo et al. (*Biochemistry*, 37,

(1998), 10928-10936) who made loop chimaeras of HIV-1 and HIV-2 protease to try to understand determinants of inhibitor-binding specificity.

Of particular relevance are cases where the binding cavity is modified so as to provide a surrogate system to obtain structural information. Thus Ikuta et al. (*J. Biol. Chem.*, 276, (2001), 27548-27554) modified the binding cavity of cdk2, for which they could obtain structural data, to resemble that of cdk4, for which no X-ray structure is currently available. In this way they were able to obtain protein/ligand structures from the chimaeric protein which were useful in cdk4 inhibitor design.

Thus from a knowledge of the structure and residues of the binding cavities of ADC described herein, a person skilled in the art could modify a non-ADC protein to produce a chimaeric ADC protein having a binding cavity or cavities which mimics those of ADC. The chimaeric protein could then be used to obtain information on compound binding through the determination of chimaeric protein/ligand complex structures (which may be characterized using the ADC crystal structure).

This strategy could readily be applied to proteins that exhibit high sequence homology with ADC, whether or not the proteins have overlapping substrate specificities with ADC. The proteins may also come from different species.

The determination by X-ray crystallography of the three-dimensional structures of such chimaeric proteins relies on the ability of the chimaeric proteins to yield crystals that diffract at high resolution. Thus if high quality crystals of the unmodified protein can already be produced, an aim could be to modify the inside part of the protein to produce a new substrate binding cavity which mimics ADC without modifying the outside shell of the protein that allows the protein to crystallize.

The substrate specificity of an enzyme generally relies on only a limited number of residues located in non-contiguous parts of the polypeptide chain. Thus this aspect of the invention provides a chimaeric protein having a binding cavities for L-aspartate, the binding cavity providing a plurality of atoms which interact with L-aspartate and which correspond to selected ADC atoms in the ADC binding cavity for L-aspartate, the relative positions of the plurality of atoms corresponding to the relative positions, as defined by Table 1, of the selected ADC atoms, wherein either or both of binding site nos. 1 and 9 defined by Table 2 provide one or more of the selected ADC atoms. Typically, the plurality of atoms are linked by at least one amino acid residue which is not present in the equivalent position in ADC. Generally, smaller proteins are easier to manipulate, crystallise etc., and so preferably the chimaeric protein contains less than 90% (more preferably less than 75% or 50%) of the number of residues contained by ADC.

Typically the plurality of atoms would derive from respective amino acid residues, and thus the minimal mutation that would usually be required to convert a protein into a ADC chimera according to this aspect involves the selection of at least two residues from Table 1. These mutations could be introduced by site-directed mutagenesis e.g. using a Stratagene QuikChange™ Site-Directed Mutagenesis Kit or cassette mutagenesis methods (see e.g. Ausubel et al., eds., *Current Protocols in Molecular Biology*, John Wiley & Sons, Inc., New York, and Sambrook et al., *Molecular Cloning: a Laboratory Manual*, 2nd ed., Cold Spring Harbor Laboratory Press, Cold Spring Harbor, NY, (1989)).

In practice, it will be desirable to provide a sufficient number of atoms in the chimaeric protein which interact with L-aspartate. Thus preferably the binding cavity of the protein

will provide at least 5 or 10, more preferably at least 50 and even more preferably at least 100 atoms which correspond to selected ADC atoms in the ADC binding cavities for L-aspartate.

By identifying conditions under which high quality crystals of fully processed ADC can be produced (i.e. crystals which can diffract X-rays for the determination of atomic coordinates to a resolution of better than 2Å), the present invention facilitates the identification of modulators of ADC activity.

Thus a further aspect of the present provides a method of assessing the ability of a candidate modulator to interact with ADC which comprises:

obtaining or synthesising said candidate modulator;

forming a crystallised complex of fully processed ADC and said candidate modulator, the complex diffracting X-rays for the determination of atomic coordinates of the complex to a resolution of better than 2Å; and

analysing the complex by X-ray crystallography to determine the ability of the candidate modulator to interact with ADC.

The step of analysing the complex may involve e.g. phasing, molecular replacement or calculating a Fourier difference map of the complex as discussed above. However, with the high resolutions obtainable with the crystal, it can also be possible to determine the ability of the candidate modulator to interact with ADC merely by comparing the intensities and/or positions of X-ray diffraction spots from the complex with e.g. diffraction spots of uncomplexed ADC or a previously identified ADC-ligand complex. Thus the step of analysing the complex may involve analysing the intensities and/or positions of X-ray diffraction spots from the complex to determine the ability of the candidate modulator to interact with ADC.

The crystallised complex may be formed by e.g. crystal soaking or co-crystallisation.

In another aspect, the invention includes a compound which is identified as an agent compound (such as an inhibitor of ADC) for modulating ADC activity by the method of one the previous aspects.

Having obtained and characterized a modulator compound according to the invention, the invention further provides a method for modulating the activity of ADC which method comprises:

providing fully processed ADC under conditions where, in the absence of modulator, the ADC is able to synthesize β-alanine from L-aspartate;

providing a modulator compound; and

determining the extent to which the activity of fully processed ADC is altered by the presence of said compound.

Following identification of an agent compound it may be manufactured and/or used in preparation, i.e. manufacture or formulation, of a composition such as a medicament, pharmaceutical composition or drug. These may be administered to individuals.

Thus, the present invention extends in various aspects not only to an agent compound as provided by the invention, but also a pharmaceutical composition, medicament, drug or other composition comprising such an agent compound e.g. for treatment (which may include preventative treatment) of a disease such as a microbial infection; a method comprising administration of such a composition to a patient, e.g. for treatment of a disease such as a microbial infection; use of such an agent compound in the manufacture of a composition for administration, e.g. for treatment of a disease such as a microbial infection; and a method of making a pharmaceutical composition comprising admixing such an agent compound with a

pharmaceutically acceptable excipient, vehicle or carrier, and optionally other ingredients.

Thus a further aspect of the present invention provides a method for preparing a medicament, pharmaceutical composition or drug, the method comprising:

identifying an ADC modulator molecule (which may thus be termed a lead compound) by a method of any one of the other aspects of the invention disclosed herein;

optimising the structure of the modulator molecule; and

preparing a medicament, pharmaceutical composition or drug containing the optimised modulator molecule.

By "optimising the structure" we mean e.g. adding molecular scaffolding, adding or varying functional groups, or connecting the molecule with other molecules (e.g. using a fragment linking approach) such that the chemical structure of the modulator molecule is changed while its original modulating functionality is maintained or enhanced. Such optimisation is regularly undertaken during drug development programmes to e.g. enhance potency, promote pharmacological acceptability, increase chemical stability etc. of lead compounds.

In another aspect, the present invention provides systems, particularly a computer system, intended to generate structures and/or perform rational drug design for ADC, or complexes of ADC with a potential modulator; the systems containing computer-readable data comprising at least one of: (a) atomic coordinate data according to Table 1, said data defining the three-dimensional structure of fully processed ADC; and (b) structure factor data for ADC, said structure factor data being derivable from the atomic coordinate data of Table 1.

For example the computer system may comprise: (i) a computer-readable data storage medium comprising data storage

material encoded with the computer-readable data; (ii) a working memory for storing instructions for processing said computer-readable data; and (iii) a central-processing unit coupled to said working memory and to said computer-readable data storage medium for processing said computer-readable data and thereby generating structures and/or performing rational drug design. The computer system may further comprise a display coupled to said central-processing unit for displaying said structures.

In a further aspect, the present invention provides computer readable media with at least one of: (a) atomic coordinate data according to Table 1 recorded thereon, said data defining the three-dimensional structure of fully processed ADC; and (b) structure factor data for ADC recorded thereon, the structure factor data being derivable from the atomic coordinate data of Table 1.

By providing such computer readable media, the atomic coordinate data can be routinely accessed to model fully-processed ADC. For example, RASMOL (Sayle *et al.*, *Trends in Biochemical Sciences*, Vol. 20, (1995), 374) is a publicly available computer software package which allows access and analysis of atomic coordinate data for structure determination and/or rational drug design.

On the other hand, structure factor data, which are derivable from atomic coordinate data (see e.g. Blundell *et al.*, *Protein Crystallography*, Academic Press, New York, London and San Francisco, (1976)), are particularly useful for calculating e.g. difference Fourier electron density maps.

A further aspect of the invention provides a method of providing data for generating structures and/or performing rational drug design for ADC, or complexes of ADC with a potential modulator, the method comprising:

(i) establishing communication with a remote device containing computer-readable data comprising at least one of: (a) atomic coordinate data according to Table 1, said data defining the three-dimensional structure of fully processed ADC; and (b) structure factor data for ADC, said structure factor data being derivable from the atomic coordinate data of Table 1; and

(ii) receiving said computer-readable data from said remote device.

Thus the remote device may comprise e.g. a computer system or computer readable media of one of the previous aspects of the invention. The device may be in a different country or jurisdiction from where the computer-readable data is received.

The communication may be via the internet, intranet, e-mail etc. Typically the communication will be electronic in nature, but some or all of the communication pathway may be optical, for example, over optical fibres.

Brief Description of the Drawings

Fig. 1 shows schematically the pathway for the biosynthesis of pantothenic acid.

Fig. 2 shows schematically the mechanism for the processing of ADC.

Figs. 3a to e show the respective structures of ADC ligands and also show how the ligands interact with three significant functional regions of the ADC binding cavity, i.e. the C_α and C_β pockets and the Pvl25A/imine species: the C_α and C_β pockets are shown schematically, whereas the Pvl25A/imine species is given in chemical notation.

Fig. 4 shows the previously proposed (Ramjee *et al.*) catalytic mechanism of ADC.

Figs. 5a and b show respectively ribbon representations of fully processed ADC tetramer viewed perpendicularly to and along its fourfold axis.

Figs. 6a to c show stick model stereo representations of the ADC binding cavity and respective bound ligands, with the observed electron densities of Tail24A in wire-frame: in Fig. 6a the ligand is α-methyl aspartate and Tail24A is in the C-state, in Fig. 6b the ligand is L-aspartate and Tail24A is in the H-state, and in Fig. 6c the ligand is reductively bound β-alanine and Tail24A is in the O-state. Also shown in wire-frame in Fig. 6b is an observed negative difference density which appears over the ligand atoms after refinement of the complete structure and which was modelled as three water molecules. The prominent wire-frame density in Fig. 6c between the ligand and Gly24A was modelled as sulphate.

Figs. 7a to c show plots (in thin line) of side chain temperature factor for the subunit A residues of respectively the α-methyl aspartate, L-aspartate and reductively bound β-alanine complexes. For reference, in each case the native side chain temperature factor is also plotted (in thick line).

Fig. 8 shows schematically the residues and interactions of the βCO_2 binding pocket (interatomic distances are in Å).

Figs. 9a to d show schematically the four steps in the proposed decarboxylation catalytic process (interatomic distances are in Å).

Detailed Description of the Invention

The present invention is founded at least partly on the production of fully processed ADC, the characterisation of the ADC binding cavity and the determination of a likely mechanism for aspartate decarboxylation.

In order to determine this mechanism and the binding site interactions the structures of several ADC-ligand complexes

were solved. The ligands which were studied were: L-aspartate (hereinafter referred to as *Sbst*), β-alanine (*Prod*), reductively bound β-alanine (*rβAla*), α-methyl aspartate (*MeAsp*), 3-amino-4-methylpentanoic acid (i.e. β-isopropyl-β-alanine, *isoA*). The structures of the respective ligands are shown in Figs. 3a to e. The structure of the uncomplexed protein (*Nat*) was also solved under identical conditions to those used for the ligand complexes, to enable better structural comparison with the complexes.

We have found that elements of the model of aspartate binding originally proposed by Albert *et al.* are correct: *Sbst* βCO_2 (i.e. the L-aspartate carboxylate group furthest from the amine group, αCO_2 being the other L-aspartate carboxylate group) is in a well-defined pocket and forms a salt-bridge with the guanidyl group of Arg54D, the salt-bridge being stacked over the aromatic ring of Trp47D; *Sbst* αCO_2 is situated in another well-defined pocket; while an imine bond formed from the *Sbst* amine group and the Pvl25A ketone closest to the split in the π-chain group results in an imine-amide intermediate. Fig. 4, which shows the previously proposed (Ramjee *et al.*) catalytic mechanism, illustrates the imine-amide intermediate. Three significant functional regions of the binding cavity may be identified: (i) Pvl25A which is needed to form the imine species, (ii) a binding pocket for *Sbst* βCO_2, and (iii) a binding pocket for *Sbst* αCO_2. These regions are illustrated in Figs. 4a to f which also show schematically how the ligands interact with these regions.

However, contrary to expectation, the βCO_2-guanidyl salt bridge is significantly non-planar, although an approximate plane may be constructed (RMS deviation between 0.16 and 0.23 Å). Also, although the atoms of the imine species in the four complexes formed respectively from *MeAsp*, *IsoA*, *Prod* and *Sbst* are nearly planar (the RMS deviation is between 0.02 and

0.06 Å), even this species does not appear completely planar, but has a slight rotational deviation (175-178°) around the imine-amide C-C bond (i.e. what was previously the pyruvoyl inter-oxygen C-C bond).

A significant advance over the model proposed by Albert *et al.* relates to the residues of Tail24A. Not only have we been able to determine the positions of these residues (except for Glu23A which was disordered in all the structures we studied as well as in the structure reported by Albert *et al.*) for *Nat* and the various ADC-ligand complexes, but we have determined the crucial role Tail24A plays in asparate decarboxylation.

Solving the Crystal Structures

1. Abbreviations

IPTG, isopropyl-β-D-thioglactopyranoside; SeMet, L-selenomethionine; DTT, dithiothreitol; ATP, adenosine triphosphate; PMSF, phenylmethylsulphonyl fluoride; HEPES, *N*-2-hydroxyethylpiperazine *N'*-2-ethanesulphonic acid; PEG_{400} /$_{4000}$ /$_{8000}$, polyethylene glycol average MW 400/4000/8000; MPD, 2-methyl-2,4-pentanediol.

2. Materials and Methods

All the compounds used were obtained from Sigma, P.O.Box 14508 St. Louis, MO 63178, USA, with the following exceptions. Liquid and solid LB medium, Yeast Extract, Bactotryptone, Agar and the DIFCO Amino Acid Assay Medium were obtained from DIFCO Laboratories, Detroit, MI 48232-7058, USA. IPTG, HEPES and DTT were obtained from Melford Laboratories Ltd., Chelsworth, Suffolk IP7 7LE, UK. PEG_{4000}, PEG_{8000}, and MPD were purchased from Fluka Chemie AG, Messerschmidt Strasse 17, D-89231, Neu-Ulm, Germany. Ethanol and ethylene glycol were obtained from Fischer Scientific UK Ltd., LE11 5RG, UK. 3-Amino-4-methyl-

pentanoic acid was obtained from ACROS, New Jersey, USA. α-methyl aspartate was synthesised in-house. All chromatography matrices were obtained from Pharmacia Biotech (now Amersham Pharmacia Biotech), Uppsala, Sweden.

Chromatography at 4 °C was performed using a Pharmacia FPLC system. At 37 °C the Pharmacia Äkta Explorer system was used. Concentrators were either (for volumes below 4 ml) Ultrafree™ centrifugal concentrators from Millipore Corporation, Bedford, MA 01730, USA; or (for larger volumes) the Amicon™ Ultrafiltration Cell, manufactured by Amicon Inc., Beverley, MA 01915, USA. Linbro™ plates were obtained from ICN Biomedicals Inc., 1263 South Chillicothe Rd., Aurora, Ohio, 44202. Qplate II™ and CrystalCap™ accessories were supplied by Hampton Research, 27632 El Lazo Road, Suite 100, Laguna Niguel, CA 92677-3913, USA.

To prepare the ADC, a glycerol stock of *E. coli* SJ16::pDKS1 (Ramjee *et al.*) was used to seed 1l of Terrific Broth containing 60 mg/ml ampicillin and 80 mg/ml IPTG. Growth was continued for 16 hours and approximately 6 g of stationary phase cells were harvested by centrifugation at 4000 g for 15 minutes, resuspended in 15 ml of buffer containing 10 mM Tris pH 8.0 and lysed by two passages through a French Press.

The crude lysate was centrifuged at 10 000 g for 30 minutes and filtered using 0.22 micrometer nitrocellulose before loading at 1 ml/min onto a Q-Sepharose Fast Flow column (Pharmacia 17-0510-01, 10 x 2 cm diameter, 30 ml matrix volume). The column was washed with 25 ml of 10 mM Tris pH 8.0. Protein was eluted using the same buffer with a zero to 1 M gradient of KCl and 2.5 ml fractions collected.

Fractions containing ADC were identified using Tricine SDS-PAGE (Schagger *et al.*, *Analytical Biochemistry*, 166, (1987), 368-379), pooled and dialysed for 16 hours and 2 hours

in 5 l of buffer containing 10 mM Tris pH 6.8. Pooled fractions were loaded onto a hydroxyapatite column (5 g Bio Rad HTP Hydroxyapatite No. 130-0420, in a 2.5 x 3.6 cm matrix volume) and eluted with a gradient of 10 to 500 mM KH_2PO_4 pH 7.0. Fractions containing ADC were identified using SDS-PAGE as before, pooled, and concentrated by ultrafiltration (Amicon centriprep 10 concentrators repeatedly centrifuged at 3000 g for 20 min) to approximately 10 mg/ml purified ADC. Approximately 5 mg ADC was obtained per gram of cells.

The ADC was stored at 4 °C for several weeks during which time autocatalytic processing occurred to form fully processed ADC with four binding site pyruvoyl groups per tetramer.

3. Protein Crystallisation

The protein was transferred to 25 mM HEPES buffer at pH 7.5 by repeated dilution and concentration using an Ultrafree™ filter. The final protein concentration was between 6 and 10 mg/ml, as judged by its theoretical extinction coefficient e_{280} = 1.09 ml/mg (see Gill *et al.*, *Analytical* Biochemistry, 182, (1989), 319-326). The crystallising solution was unbuffered $(NH_4)_2SO_4$ at concentrations of between 1.6 and 2.4 M. Equal volumes of protein and crystallisation solutions (2-10 ml) were placed on siliconised cover slides and sealed in wells containing the crystallisation solution (1 ml), in Linbro™ or Qplate II™ plates for vapour diffusion crystallisation as hanging or sitting drops respectively (as described by Sawyer *et al.*, in *Crystallization of Nucleic Acids and Proteins*, ed. Ducroix and Giege, 225-289, John Wiley & Sons, New York, 1992). The protein crystallised both at 4 and 19 °C, although the volume ratio of crystallisation to protein solution needed changing to 2:1 when at 4 °C. Crystals formed within 1-7 days, depending on temperature and component concentrations. Typical crystals were clear

hexagonal pyramids, but frequently grew on a surface so that the pyramid was only half formed. Crystals as long as 0.6 mm were grown. Growth in sitting drops or alternatively at 4 °C yielded the largest crystals.

The condition used here differed substantially from those used by Albert *et al.*, where PEG_{4000} was used with acetate buffer at pH 4.8. The pH of the HEPES buffer protein solution and the protein concentration was apparently significant in enabling the crystallisation of fully processed ADC in the present method.

4. Preparation of Crystals of ADC-Ligand Complexes

Six different ligands were used for ADC-ligand complexes. The crystals of ADC were robust and appeared to withstand high solution concentrations of the ligands.

Sbst: Protein crystals were transferred to a crystallisation solution (1.9 M $(NH_4)_2SO_4$) containing 0.5 M *Sbst*. The solution was buffered to pH 4.5 with 50 mM NaAcetate. The soaking time was 10 minutes prior to mounting.

Prod: Protein crystals were transferred to a crystallisation solution (1.9 M $(NH_4)_2SO_4$) containing 0.5 M *Prod*. The soaking time was 10 minutes prior to mounting.

rβAla: *Prod* was reductively bound to ADC in solution using $NaCNBH_3$, using the method described by Ramjee *et al.*, but substituting β-alanine for L-aspartate. The adduct was concentrated and crystallised as for the native protein.

MeAsp, *isoA*: These compounds were added in solid form to separate drops containing crystals of ADC, and left for 10-20 minutes before mounting.

The *Nat* and complex crystals were placed in crystallisation solution containing 25% glycerol for between 10-300 seconds. Each crystal was then scooped up in a cryoloop smaller than the crystal using the CrystalCap™

system (Hampton Research) Within 3 seconds the crystal was either plunged into liquid nitrogen, or flash-cooled in a stream of nitrogen gas at 100 K, and kept at low temperature (< 110 K) until after data collection.

5. Data Collection

All the ligand-complex data were collected with a Raxis IV detector using copper K_α radiation from a Rigaku rotating anode generator, with crystals cooled to 100 K. The native dataset was collected on Station 9.6 at the Daresbury Laboratory Synchrotron Radiation Source with an ADSC Quantum 4 detector. Reflections were integrated with either *DENZO* (Otwinwski *et al.*, *Processing of X-ray diffraction data collected in oscillation* mode, in *Methods in Enzymology*, Vol. 276, ed. Carter and Sweet, Academic Press, 1997) or *MOSFLM* (Leslie, *Joint CCP4 and EESF-EACMB Newsletter on Protein Crystallography*, Vol.26, Daresbury Laboratory, UK); data were scaled and merged using either *SCALEPACK* (Otwinwski *et al.*) or *SCALA* (Collaborative Computational Project 4 - CCP4. The CCP4 Suite: Programs for Protein Crystallography, *Acta Crystallographica*, D50, (1994), 760-763); and intensities were converted to amplitudes using *TRUNCATE* (CCP4). Data quality statistics are given in Table 3.

During data collections from *MeAsp*, *rβAla*, *Prod*, and *Sbst*, the 2θ-angle (Table 3) needed changing from the standard 0° setting to enable recording of the high angle data on the 30 cm detector surface while allowing a crystal-detector separation where reflections did not overlap due to the long crystallographic c-axis, high mosaicity, and large beam divergence of the home X-ray source. In spite of the high symmetry of the reciprocal lattice (6/mmm), such a detector setting required the collection of oscillation data from at least two crystal orientations to enable acceptable (but even

then not complete) coverage of reciprocal space. The data for *Sbst* were the least complete due to premature crystal destruction.

6. Refinement and Model Building

Refinement was performed similarly for all crystal structures. The crystallographic cell parameters agreed closely with those of the published structure of Albert *et al.*, which was therefore intially used directly in the refinement, thereby avoiding an explicit molecular replacement search. The *MeAsp* structure was solved relatively early in this way and for some of the later complexes the *MeAsp* structure was used as the starting model. Tail24A and Pvl25A were excluded from the initial rigid-body refinement and 12 cycles of restrained isotropic refinement with *REFMAC* (Murshudov *et al.*, *Acta Crystallographica*, D53, (1997), 24-255). Using map coefficients generated by *REFMAC*, σ_A-weighted (Read, *Acta Crystallographica*, A42, (1986), 140-149) $2mF_o$-DF_c and difference maps were calculated and manipulated using CCP4 and Uppsala Software Factory (G.J. Kleywegt, Dept. of Cell and Molecular Biology, Uppsala University, Biomedical Centre, Box 596, SE-75124 Uppsala, Sweden) programs, and examined in *O* (Jones *et al.*, *Acta Crystallography*, A47, (1991), 110-119), which was used for all model rebuilding. The ligand species were built into the clearly identifiable difference density, and errors corrected in the rest of the model. At this stage the residues of Tail24A were only built, where possible, after a further round of refinement, and ordered solvent molecules were automatically added by alternating cycles of *ARP* (Perrakis *et al.*, *Acta Crystallographica*, D55, (1999), 1765-1770) and *REFMAC* until convergence of the R_{free} model-data residual (Brunger *et al.*, *Acta Crystallographica*, D54, (1992), 905-921).

For each model, omit maps for Tail24A were recalculated using the program *BUSTER* (Bricogne, *Methods in Enzymology*, 276, (1993), 361-423) in its implementation with *TNT* (Tronrud, *Methods in Enzymology*, 277, (1997), 306-319). The refined structure from *REFMAC*, with Tail24A omitted along with any solvent molecules in the area, was briefly re-refined with optimised bulk solvent parameters, followed by Maximum Entropy partial structure completion and calculation of σ_A-weighted mF_o-DF_c difference maps. Tail24A was modelled into all structures (in the absence of good density then by comparison with well-ordered structures) and refined to convergence with *BUSTER/TNT*. The refinement convergence and some model quality indicators are summarised in Table 4.

The standard Engh & Huber (Engh *et al.*, *Acta Crystallographica*, A47, (1991) 392-400) parameters were used as geometric restraints for the ligands, where available. All structures, apart from the *rβAla* and *MeSuc* complexes and *Nat*, were defined to contain a planar imine-amide species, which is not represented in those parameters, and the relevant bond-lengths and angles were taken from the Cambridge Structural Database (CSD, Allen *et al.*, *J. of Chemical Information and Computer Sciences*, 31, (1991), 187-204). The pyruvoyl in *Nat* was modelled in the *cis* conformation.

The different models agreed closely (between 0.1 and 0.2 Å RMS deviation over all C_α-atoms), with differences limited to the binding cavity. The various soaked ligands did bind and were clearly visible.

Structural Characterisation

1. *Nat*

Tail24A residues were very well ordered, along with a solvent molecule between Tyr22A and Pvl25A. There was a prominent density of uncertain origin deeper in the binding

cavity in the substrate βCO_2 pocket between Pvl25A and Arg54D. It was modelled as solvent. Table 1 provides the atomic coordinates of the *Nat* structure.

Unlike the partially processed enzyme (which only has a pseudo-fourfold rotation axis and at most three binding cavities), the fully processed ADC tetramer has a crystallographic fourfold rotation axis and four binding cavities. This significantly simplifies the analysis of X-ray experiments (e.g. for the determination of the structures of the complexes discussed below), the higher symmetry of the fully processed tetramer facilitating the interpretation of diffraction data and the additional binding cavity increasing the intensity of reflections from binding cavities.

A ribbon representation of the fully processed tetramer is shown viewed perpendicularly to the four-fold axis in Fig. 5a and along the fourfold axis in Fig. 5b.

2. *MeAsp, IsoA, Prod*

These complexes had the cleanest density. The ligand positions were evident, and Tail24A was very well ordered, with no spurious density peaks. In *Prod*, there was a solvent molecule between Tyr22A and the Pvl25A/ligand adduct, in the same position as the αCO_2Me and isopropyl groups of *MeAsp* and *IsoA*. This position corresponds to the substrate αCO_2 pocket.

3. *rβAla*

The reduced β-alanine was located with ease, however Tail24A appeared more disordered. Only His21A and Tyr22A were defined, but by very weak densities. In the substrate αCO_2 pocket there was a very prominent difference density feature. There is a significant likelihood that it is due to a sulphate ion - a crystallisation precipitant which has bound in this site. Sulphate matched the density reasonably well, and (at

occupancy = 0.5) refined to B-factors of around 47 and 37 Å^2 in the respective A and D subunits, which compared favourably with some of the less well-ordered parts of the structure. The two negative sulphate charges would be accommodated by $N_{\zeta Lys9D}$ and the reduced nitrogen of the ligand (N_{Lig}), both of would be protonated and positive at the pH of crystallisation. The absence of such a sulphate in *Prod* may be explained by the different orientation of N_{Lig}, which in *rβAla*, points towards the putative sulphate, but in *Prod* towards the Asn72A mainchain.

4. *Sbst*

Contrary to the other complexes, two crystallographically unique conformations, **Y** and **Z**, of ADC were observed in the asymmetric unit (with respect to the respective tetramer π-chains, conformation **Y** was observed in binding cavities D/A and B/C, and conformation **Z** in cavities A/B and C/D). These two conformations showed distinct differences in their respective binding cavities and appeared to correspond to different stages of decarboxylation. The difference densities for the ligands showed that neither conformation was as well ordered as ADC in the complexes with the other ligands. In both conformations there were breaks in the observed electron densities, but this may be a crystallographic artifact caused by incompleteness of the *Sbst* dataset. Of course, in view of the fact that *Sbst* undergoes decarboxylation by ADC it is not surprising that well-defined densities were not obtained.

Tail24A differed between the conformations, but in both it was visible only at low map contour levels and therefore accompanied by much spurious density which is unsurprising, since we expect to see a superposition of reaction states in the *Sbst* complex. With conformation **Z**, density is relatively convincing; while with conformation **Y**, it is significantly

less well ordered, with a break in the C_α density of Tyr22A and a poorly defined Gly24A. The orientation of the terminal carboxylate group of Tail24A with conformation **Y** is different from that of the other structures, pointing out of the binding cavity rather than down at the amino group of Lys9D. A large difference density feature around Lys9D and Tyr58A was seen, at a higher map contour level, to consist of three separated peaks, and was therefore modelled as three water molecules.

So three states of Tail24A may be distinguished: the C- (closed), O- (open), and H- (half-closed) states. The C-state (seen in complexes with *Nat*, *MeAsp*, *IsoA*, and *Prod* is a conformation in which Tail24A blocks off the binding cavity and is well ordered, the terminal carboxylate of Gly24A interacting with Lys9D. In the O-state (seen in the complex with *rβAla*) Tail24A is largely disordered and the binding cavity is exposed. In the H-state (seen with ADC conformation **Y** in the complex with *Sbst*) most of Tail24A has the C-state conformation, except the terminal carboxylate of Gly24A which does not interact with Lys9D.

Table 2 (see below) provides the coordinates and binding interactions of binding sites within the binding cavity. The C-, H- and O-states are respectively illustrated in Figs. 6a to c which show stereo representations of the binding cavity together with the observed electron density of Tail24A. In Fig. 6a the ligand is *MeAsp*, in Fig. 6b it is *Sbst* (in the complex with ADC conformation **Y**), and in Fig. 6c it is *rβAla*.

Figs. 7a to c show plots (in thin line) of side chain temperature factor (*B* in Table 4) for the subunit A residues of respectively the *MeAsp*, *Sbst* and *rβAla* complexes, i.e. the C-, H-, and O-states. For reference, in each case the *Nat* side chain temperature factor is also plotted (in thick line). Significant is the height of the main peak (corresponding to

the residues of Tail24A) which increases in height as Tail24A progresses from the C-state to the O-state. This implies that in the O-state Tail24A is less strongly constrained to a particular conformation, i.e. Tail24A is more mobile. So although complexes having the respective states may be modelled by refined structures in which Tail24A adopts similar conformations, the higher *B*-factors allotted to the side chains of Tail24A in the O-state are evidence of an increased indeterminacy in the position of Tail24A. This is consistent with increased exposure of the binding cavity in the O-state.

Aspartate Decarboxylation

An elaborated version of the Albert *et al.* explanation for initial binding of the substrate into the binding cavity requires only minimal distortion of the residues of the two adjacent π-chain subunits. The guanidyl group of Arg54D is ideally positioned in a deep, hydrophobic pocket (Trp47D, Phe55A, Ala75A) to form a strong, directed salt bridge with the negatively charged aspartate βCO_2 group. The resulting aromatic stacking with Trp47D is known to be a favourable type of interaction (Westhead *et al.*, *Trends in Biochemical sciences*, 23, (1998), 35-36). The βCO_2 binding pocket is shown schematically in Fig. 8.

N_{Lig} (i.e. in this case the L-aspartate nitrogen atom) is thus placed at a suitable distance for imine formation above the Pvl25A ketone closest to the split in the π-chain. The substrate αCO_2 group is then positioned above the plane of the newly-formed imine-amide group in the hydrophobic environment of Tyr22A, Tyr58A and Ile60A, and the Pvl25A methyl group. This provides the non-polar incentive to neutralise the negatively-charged substrate αCO_2 and drive decarboxylation; the resulting negative charge on the adjacent (C_α) substrate carbon being dispersed over the planar imine-amide group and

beyond via hydrogen bonding between the oxygen of the remaining Pvl25A ketone and strands β5 and β1 of subunit A and solvent molecules. The negative charge is finally neutralised by protonation of the substrate C_α carbanion.

However, this mechanism does not explain how the base, which must be available to protonate the C_α carbanion, is earlier prevented from stabilising the negatively-charged substrate αCO_2, thereby preventing decarboxylation. Also, the position of the Tyr22A group varies with the position of Tail24A, and so is only available to provide a hydrophobic environment for the αCO_2 group in certain positions of Tail24A.

We therefore propose the following four-step catalytic process which takes account of these factors:

(1) Tail24A flips from the C- to the O-state to allow the substrate molecule to enter the binding cavity. The substrate βCO_2 positions itself in the Trp47D, Phe55A, Ala75A hydrophobic pocket and N_{Lig} reacts with Pvl25A to form the imine-amide group, as described above. Tail24A then undergoes an O- to H-state transition whereby Tyr22A completes the hydrophobic pocket around the substrate αCO_2 group.

(2) Tail24A undergoes an H- to C-state transition whereby the terminal carboxylate group of Gly24A neutralises the positive charge on Lys9D which had previously stabilised the substrate αCO_2 group.

(3) The substrate αCO_2 group undergoes decarboxylation.

(4) The decarboxylated substrate C_α carbanion is protonated and Tail24A opens to allow the carbon dioxide molecule to escape.

Steps (1) to (4) are illustrated schematically in Figs. 9a to d, and are described in more detail below.

Step (1)

The detailed mechanism by which Tail24A flips from the C- to the O-state to allow the substrate molecule to enter the

binding cavity, is not entirely clear. Possibly the steric and electrical presence of the substrate molecule is sufficient to force away the aromatic hydrophobic Tyr22A sidechain (and thus the rest of Tail24A) in the same way that the sulphate ion in the *rβAla* complex apparently forces Tail24A into the O-state. Note the position of Asp19A means that it is not possible simply to rotate the Tyr22A sidechain out of the binding cavity while maintaining the Tail24A mainchain in the C-state; the whole of Tail24A has to move away.

In any event, once the substrate is completely bound, through both βCO_2 and the imine species, the position and orientation of αCO_2 induce the H-state. There are four interactions which fix Tyr22A into this conformation, one to the substrate, three within the enzyme: O_{Tyr22A} hydrogen bonds to His11D, and the Tyr22A sidechain bonds with Asp19A and Asn72A. These two interactions arise from the electric dipole of the Tyr22A phenyl π-bond system which carries a fractional negative charge above, and a fractional positive charge equatorial to, the ring: the protons of the Asn72A sidechain amide interact with the former, the negative charge on Asp19A with the latter. The same effect allows the fourth Tyr22A interaction, which is the approach of the hydrophobic phenyl ring to the negatively charged substrate αCO_2 group. This completes around αCO_2 the hydrophobic pocket consisting of Tyr22A , Tyr58A, Ile60A (not shown in Figs. 9a to d) and the pyruvoyl methyl carbon.

The αCO_2 group also forms a hydrogen bridge to the positively charged Lys9D, forming the latter's third hydrogen bond (along with Tyr58A and His11D). At this stage, the negative Gly24A terminal carboxylate does not bind to Lys9D, and instead it has to adopt the conformation seen in conformation **Y**.

The two equatorial phenyl-carboxylate interactions (substrate αCO_2 and Asp19A) involve the formally uncharged (see Fig. 8a) oxygens of the carboxylates, since the charged oxygens interact with N_{ZLys9D} and N_{His21A} respectively, both of which are better able to accommodate the negative charge than the only fractionally positive charge on the aromatic ring.

Step (2)

Because of its linkage to Tyr22A, the negatively charged Gly24A carboxylate is drawn into forming a salt bridge with the closest positive charge, which is that on N_{ZLys9D}. Tail24A is now in the C-state. The differing observations in the two ADC conformations with *Sbst* illustrate this competition for N_{ZLys9D}: in conformation **Y**, the substrate appears to be more clearly present than in **Z**, which suggests that **Y** represents a less advanced stage in the catalytic process. This is also consistent with Gly24A being relatively poorly ordered and not bound to N_{ZLys9D} (i.e. the H-state) with conformation **Y**, whereas Gly24A is more ordered and Tail24A is more nearly in the C-state with **Z**.

The formation of the C-state observed with *MeAsp* and *IsoA* is also consistent with this step of the proposed mechanism. Like *Sbst*, *MeAsp* and *IsoA* are held in the binding cavity by the formation of the imine species and the favourable positioning of their carboxylate groups in the substrate βCO_2 binding pocket. However, unlike *Sbst*, neither *MeAsp* nor *IsoA* has a decarboxylatable αCO_2 group. Instead each has a relatively hydrophobic group (respectively αCO_2Me and isopropyl) which is stable in the αCO_2 hydrophobic binding pocket and does not hydrogen bond to N_{ZLys9D}. Consequently, the N_{ZLys9D}-Gly24A carboxylate salt bridge is favoured and Tail24A is immobilised in the C-state.

Prod, like *MeAsp* and *IsoA*, is held in the binding cavity by the formation of a imine species and the favourable positioning of its carboxylate group into the βCO_2 binding pocket. However, with *Prod* the $N_{\zeta Lys9D}$-Gly24A carboxylate salt bridge is favoured and Tail24A is held in the C-state because *Prod* lacks a group to interact significantly with the αCO_2 binding pocket (a solvent molecule occupies this pocket in *Prod*). Similarly, in *Nat* there is no competition from any part of a bound ligand for $N_{\zeta Lys9D}$, and so Tail24A favours the C-state.

Step(3)

The effect of the previous two steps was first to enclose αCO_2 with hydrophobic residues, and next to remove the remaining stabilising interaction with the positive $N_{\zeta Lys9D}$. This leaves the negative charge on αCO_2 unstabilised and in an unfavourable environment, and thus provides the "push" required to drive decarboxylation. The fractional positive charge equatorial to the Tyr22A sidechain is not sufficient to stabilise the negative charge. Indirect evidence of this comes from the *MeAsp* complex, in which the *MeAsp* αCO_2Me hydrophobic methyl group is oriented towards the aromatic ring of Tyr22A despite the electric dipole of the Tyr22A phenyl π-bond system.

The source of the "pull" effect, which is required to stabilise the charged, decarboxylated species, is also confirmed by the orientation of the oxygen of the remaining pyruvol ketone, which allows it to form H-bonds to the peptide bond groups between residues Val71A-Asn72A and Ala18A-Asp19A on parallel β-strands β5 and β1′ of π-chain A. The negative charge which remains on the reaction intermediate after decarboxylation is dispersed over the planar imine species, which stabilises the intermediate. This creates a net

negative charge on the electrophilic oxygen of the remaining pyruvol ketone, which in turn induces electric dipoles in the delocalised π-electrons of the two parallel amide bond systems to which it is H-bonded. This results in a stabilising dielectric effect which is further enhanced by the solvent which surrounds the amide bond between Ala18A and Asp19A. Overall the energy of the charged reaction intermediate is lowered and the reaction therefore accelerated.

Step(4)

The final step is protonation of C_α, which probably occurs rapidly before the release of CO_2 from the cavity. His11D is unlikely to be the proton donor, since both of its N-atoms are involved in H-bonds. So the remaining candidates are Tyr58A and Lys9D, both of which are within 5 Å of C_α, are part of the same H-bonding system and are exposed to solvent.

The most plausible mechanism involves both Lys9D and Tyr58A. Initially all three protons on $N_{\zeta Lys9D}$ are used in H-bonds (to Tyr58A, His11D and Gly24A) and are therefore unavailable. The OH_{Tyr58A} proton from Tyr58A, however, is available, because the proton for the H-bond between OH_{Tyr58A} and $N_{\zeta Lys9D}$ is provided by $N_{\zeta Lys9D}$. Therefore the OH_{Tyr58A} proton is transferred to the C_α, and the resulting negative charge created on OH_{Tyr58} is stabilised by the neighbouring positive charge on $N_{\zeta Lys9}$. This charge is then neutralised by transfer of the H-bonding proton from $N_{\zeta Lys9D}$ which therefore loses its positive charge. Because of this the Gly24A terminal carboxylate group debonds from $N_{\zeta Lys9D}$ and Tail24A adopts the H- or O-state, allowing the CO_2 molecule to escape from the binding cavity.

Of course, the O-state was observed with *rβAla*, but in this case the apparent reason that the Gly24A terminal carboxylate group was not bound to $N_{\zeta Lys9D}$ (thereby releasing

Tail24A from the C-state) was the steric and/or electrical effect of a sulphate ion in the αCO_2 pocket. Such an ion may be a more preferred binding partner for $N_{\zeta Lys9D}$ compared with the Gly24A terminal carboxylate.

The distance between C_α and OH_{Tyr58A} is about 4.5 Å. This may be close enough for a direct proton transfer after some side chain movement from OH_{Tyr58A} to C_α, or alternatively the CO_2 molecule may play a significant role, by transiently binding the proton during its transfer to C_α.

To summarise, a function of the somewhat elaborate Tail24A mechanism is apparently to prevent Lys9D from interfering with the process of decarboxylation until Lys9D is needed for protonation.

Structure-Based Drug Design

Determination of the mechanism of aspartate decarboxylation by ADC, and in particular the recognition of the crucial role of Tail24A, provides important information for rational design of ADC inhibitors, e.g. via computational techniques which identify possible binding ligands for the binding cavity. These techniques are discussed in more detail below.

Greer *et al.* (*J. of Medicinal Chemistry*, 37, (1994), 1035-1054) described an iterative approach to ligand design based on repeated sequences of computer modelling, protein-ligand complex formation and X-ray crystallographic or NMR spectroscopic analysis. Thus novel thymidylate synthase inhibitor series were designed *de novo* by Greer et al., and ADC inhibitors may also be designed in the this way. More specifically, using e.g. GRID (Goodford, *J of Medicinal Chemistry*, 28, (1985), 849-857.) on the solved 3D structure of ADC, a ligand (e.g. a candidate inhibitor) for ADC may be

designed that complements the functionalities of the ADC binding site. The ligand can then be synthesised, formed into a complex with ADC, and the complex then analysed by X-ray crystallography to identify the actual position of the bound ligand. The structure and/or functional groups of the ligand can then be adjusted, if necessary, in view of the results of the X-ray analysis, and the synthesis and analysis sequence repeated until an optimised ligand is obtained. Related approaches to structure-based drug design are also discussed in Bohacek *et al.*, *Medicinal Research Reviews*, 16, (1996), 3-50.

As a result of the determination of the mechanism of aspartate decarboxylation, more purely computational techniques for rational drug design may also be used to design ADC inhibitors (for an overview of these techniques see e.g. Walters et al. mentioned above). For example, automated ligand-receptor docking programs (discussed e.g. by Jones *et al.* in *Current Opinion in Biotechnology*, 6, (1995), 652-656) which require accurate information on the atomic coordinates of target receptors may be used to design candidate ADC inhibitors.

The approaches to structure-based drug design described above all require initial identification of possible compounds for interaction with target bio-molecule (in this case ADC). Sometimes these compounds are known e.g. from the research literature. However, when they are not, or when novel compounds are wanted, a first stage of the drug design program may involve computer-based *in silico* screening of compound databases (such as the Cambridge Structural Database) with the aim of identifying compounds which interact with the binding cavity or sites of the target bio-molecule. Screening selection criteria may be based on pharmacokinetic properties such as metabolic stability and toxicity. However,

determination of the mechanism of aspartate decarboxylation allows the architecture and chemical nature of the ADC binding site to be better defined, which in turn allows the geometric and functional constraints of a descriptor for the candidate inhibitor to be derived more accurately. The descriptor is, therefore, a type of virtual 3-D pharmacophore, which can also be used as selection criteria or filter for database screening.

While the invention has been described in conjunction with the exemplary embodiments described above, many equivalent modifications and variations will be apparent to those skilled in the art when given this disclosure. Accordingly, the exemplary embodiments of the invention set forth are considered to be illustrative and not limiting. Various changes to the described embodiments may be made without departing from the spirit and scope of the invention.

Table 1: Atomic structure of fully-processed native ADC

CRYST1	71.080	71.080	215.781	90.00	90.00 120.00
ORIGX1	1.000000	0.000000	0.000000		0.00000
ORIGX2	0.000000	1.000000	0.000000		0.00000
ORIGX3	0.000000	0.000000	1.000000		0.00000
SCALE1	0.014069	0.008123	0.000000		0.00000
SCALE2	0.000000	0.016245	0.000000		0.00000
SCALE3	0.000000	0.000000	0.004634		0.00000

Remarks

Atoms of tetramer subunits A and B and their associated water molecules (which are designated G) are numbered from 1 to 2075. Tetramer subunits C and D were generated by symmetry from subunits A and B, and hence the atoms of subunits C and D and their associated water molecules (which are designated H) are also numbered from 1 to 2075.

Due to lack of measured electron density, C-terminal residues 116 to 126 were not modelled for any of the tetramer subunits. Hence atoms of residues 116 to 126 do not appear in the following data lists.

The atomic coordinates provided below are for orthogonal, right-handed axes.

The following data lists provide:
Column 2: Atom no.
Column 3: Atom type
Column 4: Residue type
Column 5: Tetramer subunit
Column 6: Residue no.
Column 7: x coordinate of atom (Å)
Column 8: y coordinate of atom (Å)
Column 9: z coordinate of atom (Å)
Column 10: Occupancy
Column 11: *B*-factor (Å^2)

N.B. For water molecules, column 4 reads "WAT", column 5 reads G or H, column 6 is the no. of the water molecule, and the atomic coordinates of columns 7-9 are the coordinates of the water oxygen atoms.

Data Lists

ATOM	1	N	MET	A	1	42.243	31.537	9.436	1.00 25.25
ATOM	2	CA	MET	A	1	43.570	31.458	10.034	1.00 23.37
ATOM	3	C	MET	A	1	43.641	32.211	11.324	1.00 22.04
ATOM	4	O	MET	A	1	42.712	32.932	11.694	1.00 22.16
ATOM	5	CB	MET	A	1	44.716	31.746	9.121	1.00 26.58
ATOM	6	CG	MET	A	1	44.484	32.827	8.276	1.00 29.48
ATOM	7	SD	MET	A	1	44.383	34.380	9.083	1.00 32.96
ATOM	8	CE	MET	A	1	44.525	35.278	7.559	1.00 23.68
ATOM	9	N	ILE	A	2	44.751	32.014	11.983	1.00 14.33
ATOM	10	CA	ILE	A	2	44.972	32.564	13.345	1.00 12.86
ATOM	11	C	ILE	A	2	45.982	33.682	13.386	1.00 13.27
ATOM	12	O	ILE	A	2	47.126	33.561	12.838	1.00 12.60
ATOM	13	CB	ILE	A	2	45.444	31.363	14.210	1.00 15.76
ATOM	14	CG1	ILE	A	2	44.358	30.267	14.277	1.00 18.95
ATOM	15	CG2	ILE	A	2	45.853	31.814	15.631	1.00 15.91
ATOM	16	CD1	ILE	A	2	43.131	30.698	14.977	1.00 30.84
ATOM	17	N	ARG	A	3	45.597	34.790	14.035	1.00 11.28
ATOM	18	CA	ARG	A	3	46.492	35.952	14.142	1.00 10.27
ATOM	19	C	ARG	A	3	47.228	36.039	15.491	1.00 12.97

ATOM	20	O	ARG	A	3	46.698	35.499	16.473	1.00	11.98
ATOM	21	CB	ARG	A	3	45.661	37.245	14.103	1.00	11.24
ATOM	22	CG	ARG	A	3	44.872	37.472	12.729	1.00	11.07
ATOM	23	CD	ARG	A	3	45.819	38.078	11.695	1.00	14.19
ATOM	24	NE	ARG	A	3	44.929	38.442	10.562	1.00	12.85
ATOM	25	CZ	ARG	A	3	45.343	39.206	9.551	1.00	13.01
ATOM	26	NH1	ARG	A	3	46.582	39.576	9.415	1.00	11.87
ATOM	27	NH2	ARG	A	3	44.406	39.516	8.613	1.00	15.42
ATOM	28	N	THR	A	4	48.373	36.698	15.491	1.00	10.90
ATOM	29	CA	THR	A	4	49.176	36.964	16.738	1.00	8.73
ATOM	30	C	THR	A	4	48.907	38.466	16.993	1.00	12.54
ATOM	31	O	THR	A	4	49.309	39.358	16.137	1.00	11.96
ATOM	32	CB	THR	A	4	50.623	36.684	16.549	1.00	10.20
ATOM	33	OG1	THR	A	4	50.780	35.288	16.296	1.00	12.29
ATOM	34	CG2	THR	A	4	51.479	37.146	17.856	1.00	12.13
ATOM	35	N	MET	A	5	48.224	38.786	18.149	1.00	10.12
ATOM	36	CA	MET	A	5	47.846	40.130	18.437	1.00	10.31
ATOM	37	C	MET	A	5	48.386	40.604	19.771	1.00	13.52
ATOM	38	O	MET	A	5	48.563	39.767	20.674	1.00	14.15
ATOM	39	CB	MET	A	5	46.316	40.208	18.572	1.00	13.06
ATOM	40	CG	MET	A	5	45.503	39.690	17.370	1.00	11.30
ATOM	41	SD	MET	A	5	45.827	40.706	15.868	1.00	13.37
ATOM	42	CE	MET	A	5	45.032	42.250	16.304	1.00	14.97
ATOM	43	N	LEU	A	6	48.622	41.904	19.871	1.00	10.44
ATOM	44	CA	LEU	A	6	49.081	42.499	21.181	1.00	11.49
ATOM	45	C	LEU	A	6	47.929	42.257	22.147	1.00	13.65
ATOM	46	O	LEU	A	6	46.795	42.770	21.986	1.00	12.95
ATOM	47	CB	LEU	A	6	49.255	43.989	21.000	1.00	11.43
ATOM	48	CG	LEU	A	6	49.699	44.732	22.302	1.00	12.67
ATOM	49	CD1	LEU	A	6	51.156	44.411	22.585	1.00	13.37
ATOM	50	CD2	LEU	A	6	49.593	46.238	22.044	1.00	14.36
ATOM	51	N	GLN	A	7	48.226	41.496	23.234	1.00	12.16
ATOM	52	CA	GLN	A	7	47.239	41.216	24.275	1.00	11.30
ATOM	53	C	GLN	A	7	47.141	42.451	25.220	1.00	12.23
ATOM	54	O	GLN	A	7	46.041	42.846	25.650	1.00	11.94
ATOM	55	CB	GLN	A	7	47.746	40.036	25.107	1.00	12.62
ATOM	56	CG	GLN	A	7	46.732	39.520	26.148	1.00	14.99
ATOM	57	CD	GLN	A	7	46.688	40.421	27.435	1.00	12.25
ATOM	58	OE1	GLN	A	7	45.546	40.719	27.921	1.00	14.42
ATOM	59	NE2	GLN	A	7	47.842	40.852	27.955	1.00	13.59
ATOM	60	N	GLY	A	8	48.310	43.015	25.491	1.00	12.10
ATOM	61	CA	GLY	A	8	48.374	44.194	26.380	1.00	12.14
ATOM	62	C	GLY	A	8	49.811	44.596	26.605	1.00	11.21
ATOM	63	O	GLY	A	8	50.775	43.898	26.221	1.00	12.25
ATOM	64	N	LYS	A	9	49.985	45.756	27.260	1.00	11.80
ATOM	65	CA	LYS	A	9	51.337	46.214	27.515	1.00	12.75
ATOM	66	C	LYS	A	9	51.410	47.227	28.669	1.00	12.69
ATOM	67	O	LYS	A	9	50.401	47.872	29.006	1.00	14.09
ATOM	68	CB	LYS	A	9	51.969	46.897	26.258	1.00	16.31
ATOM	69	CG	LYS	A	9	51.366	48.231	25.859	1.00	16.10
ATOM	70	CD	LYS	A	9	52.132	48.984	24.727	1.00	15.95
ATOM	71	CE	LYS	A	9	51.406	50.282	24.423	1.00	20.48
ATOM	72	NZ	LYS	A	9	52.258	51.132	23.526	1.00	22.05
ATOM	73	N	LEU	A	10	52.615	47.337	29.208	1.00	13.44
ATOM	74	CA	LEU	A	10	52.927	48.310	30.283	1.00	13.72
ATOM	75	C	LEU	A	10	53.805	49.288	29.528	1.00	14.03
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ATOM	77	CB	LEU	A	10	53.733	47.627	31.422	1.00	13.59
ATOM	78	CG	LEU	A	10	52.977	46.504	32.112	1.00	14.77
ATOM	79	CD1	LEU	A	10	53.870	45.742	33.134	1.00	18.67

ATOM	80	CD2	LEU	A	10	51.669	47.010	32.829	1.00	15.75
ATOM	81	N	HIS	A	11	53.306	50.476	29.335	1.00	14.06
ATOM	82	CA	HIS	A	11	54.009	51.485	28.542	1.00	14.41
ATOM	83	C	HIS	A	11	54.833	52.488	29.338	1.00	18.20
ATOM	84	O	HIS	A	11	54.265	53.263	30.102	1.00	16.24
ATOM	85	CB	HIS	A	11	53.007	52.202	27.614	1.00	17.29
ATOM	86	CG	HIS	A	11	53.650	53.095	26.601	1.00	18.36
ATOM	87	ND1	HIS	A	11	54.118	52.627	25.381	1.00	20.19
ATOM	88	CD2	HIS	A	11	53.902	54.430	26.612	1.00	19.36
ATOM	89	CE1	HIS	A	11	54.652	53.629	24.711	1.00	19.59
ATOM	90	NE2	HIS	A	11	54.530	54.737	25.432	1.00	18.93
ATOM	91	N	ARG	A	12	56.146	52.442	29.124	1.00	15.16
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ATOM	93	C	ARG	A	12	57.204	53.130	31.261	1.00	16.37
ATOM	94	O	ARG	A	12	57.175	54.135	32.023	1.00	18.19
ATOM	95	CB	ARG	A	12	56.873	54.756	29.408	1.00	15.43
ATOM	96	CG	ARG	A	12	57.151	55.048	27.918	1.00	17.33
ATOM	97	CD	ARG	A	12	56.884	56.522	27.538	1.00	17.26
ATOM	98	NE	ARG	A	12	57.737	57.412	28.332	1.00	19.17
ATOM	99	CZ	ARG	A	12	58.961	57.793	28.026	1.00	24.65
ATOM	100	NH1	ARG	A	12	59.545	57.416	26.907	1.00	21.82
ATOM	101	NH2	ARG	A	12	59.630	58.580	28.874	1.00	28.03
ATOM	102	N	VAL	A	13	57.315	51.908	31.667	1.00	15.70
ATOM	103	CA	VAL	A	13	57.545	51.669	33.106	1.00	14.78
ATOM	104	C	VAL	A	13	59.069	51.826	33.262	1.00	18.42
ATOM	105	O	VAL	A	13	59.877	51.698	32.280	1.00	15.58
ATOM	106	CB	VAL	A	13	57.146	50.312	33.603	1.00	16.79
ATOM	107	CG1	VAL	A	13	55.661	50.217	33.766	1.00	18.88
ATOM	108	CG2	VAL	A	13	57.768	49.142	32.719	1.00	16.41
ATOM	109	N	LYS	A	14	59.524	52.096	34.513	1.00	15.68
ATOM	110	CA	LYS	A	14	60.941	52.258	34.789	1.00	16.45
ATOM	111	C	LYS	A	14	61.497	51.036	35.528	1.00	16.56
ATOM	112	O	LYS	A	14	60.817	50.471	36.456	1.00	16.75
ATOM	113	CB	LYS	A	14	61.161	53.498	35.659	1.00	17.97
ATOM	114	CG	LYS	A	14	62.639	53.803	35.880	1.00	20.97
ATOM	115	CD	LYS	A	14	62.866	55.127	36.574	1.00	29.18
ATOM	116	CE	LYS	A	14	62.630	56.291	35.666	1.00	32.48
ATOM	117	NZ	LYS	A	14	62.715	57.533	36.483	1.00	33.64
ATOM	118	N	VAL	A	15	62.708	50.585	35.121	1.00	13.79
ATOM	119	CA	VAL	A	15	63.339	49.420	35.746	1.00	14.02
ATOM	120	C	VAL	A	15	63.786	49.854	37.179	1.00	14.49
ATOM	121	O	VAL	A	15	64.448	50.872	37.322	1.00	14.91
ATOM	122	CB	VAL	A	15	64.579	48.948	34.960	1.00	14.72
ATOM	123	CG1	VAL	A	15	65.246	47.816	35.695	1.00	15.47
ATOM	124	CG2	VAL	A	15	64.092	48.461	33.499	1.00	15.44
ATOM	125	N	THR	A	16	63.327	49.098	38.172	1.00	14.68
ATOM	126	CA	THR	A	16	63.637	49.433	39.582	1.00	16.18
ATOM	127	C	THR	A	16	64.731	48.629	40.230	1.00	19.63
ATOM	128	O	THR	A	16	65.282	49.078	41.258	1.00	18.35
ATOM	129	CB	THR	A	16	62.365	49.292	40.416	1.00	14.13
ATOM	130	OG1	THR	A	16	61.976	47.947	40.564	1.00	17.95
ATOM	131	CG2	THR	A	16	61.253	50.204	39.873	1.00	18.04
ATOM	132	N	HIS	A	17	65.056	47.469	39.699	1.00	14.05
ATOM	133	CA	HIS	A	17	66.089	46.613	40.242	1.00	15.34
ATOM	134	C	HIS	A	17	66.664	45.687	39.129	1.00	19.86
ATOM	135	O	HIS	A	17	65.947	45.353	38.137	1.00	17.90
ATOM	136	CB	HIS	A	17	65.422	45.752	41.340	1.00	18.53
ATOM	137	CG	HIS	A	17	66.361	44.834	42.079	1.00	22.33
ATOM	138	ND1	HIS	A	17	66.377	43.473	41.869	1.00	25.17
ATOM	139	CD2	HIS	A	17	67.273	45.068	43.071	1.00	24.77

ATOM	140	CE1	HIS	A	17	67.278	42.908	42.651	1.00	25.62
ATOM	141	NE2	HIS	A	17	67.835	43.847	43.396	1.00	24.55
ATOM	142	N	ALA	A	18	67.902	45.246	39.301	1.00	16.82
ATOM	143	CA	ALA	A	18	68.552	44.311	38.349	1.00	18.95
ATOM	144	C	ALA	A	18	69.265	43.234	39.190	1.00	25.44
ATOM	145	O	ALA	A	18	69.873	43.546	40.228	1.00	26.69
ATOM	146	CB	ALA	A	18	69.508	45.039	37.431	1.00	21.19
ATOM	147	N	ASP	A	19	69.136	41.983	38.815	1.00	21.26
ATOM	148	CA	ASP	A	19	69.749	40.895	39.580	1.00	20.78
ATOM	149	C	ASP	A	19	70.278	39.807	38.655	1.00	21.60
ATOM	150	O	ASP	A	19	69.620	38.802	38.420	1.00	20.10
ATOM	151	CB	ASP	A	19	68.685	40.329	40.553	1.00	21.77
ATOM	152	CG	ASP	A	19	69.255	39.335	41.584	1.00	27.20
ATOM	153	OD1	ASP	A	19	70.469	39.097	41.617	1.00	27.06
ATOM	154	OD2	ASP	A	19	68.416	38.772	42.356	1.00	28.93
ATOM	155	N	LEU	A	20	71.500	40.003	38.200	1.00	21.47
ATOM	156	CA	LEU	A	20	72.137	39.036	37.337	1.00	21.15
ATOM	157	C	LEU	A	20	72.212	37.654	37.924	1.00	25.20
ATOM	158	O	LEU	A	20	72.017	36.677	37.212	1.00	24.39
ATOM	159	CB	LEU	A	20	73.557	39.513	36.967	1.00	21.58
ATOM	160	CG	LEU	A	20	74.383	38.693	35.995	1.00	24.50
ATOM	161	CD1	LEU	A	20	73.751	38.833	34.550	1.00	22.31
ATOM	162	CD2	LEU	A	20	75.811	39.297	36.010	1.00	24.07
ATOM	163	N	HIS	A	21	72.509	37.565	39.234	1.00	23.99
ATOM	164	CA	HIS	A	21	72.638	36.275	39.933	1.00	26.08
ATOM	165	C	HIS	A	21	71.407	35.687	40.499	1.00	29.17
ATOM	166	O	HIS	A	21	71.493	34.758	41.302	1.00	29.91
ATOM	167	CB	HIS	A	21	73.769	36.384	40.973	1.00	29.07
ATOM	168	CG	HIS	A	21	75.006	36.943	40.395	1.00	34.17
ATOM	169	ND1	HIS	A	21	75.647	36.327	39.347	1.00	37.06
ATOM	170	CD2	HIS	A	21	75.663	38.112	40.605	1.00	37.54
ATOM	171	CE1	HIS	A	21	76.679	37.059	38.967	1.00	36.64
ATOM	172	NE2	HIS	A	21	76.712	38.150	39.712	1.00	37.19
ATOM	173	N	TYR	A	22	70.251	36.223	40.095	1.00	26.33
ATOM	174	CA	TYR	A	22	68.964	35.717	40.583	1.00	27.04
ATOM	175	C	TYR	A	22	68.951	34.193	40.565	1.00	33.24
ATOM	176	O	TYR	A	22	69.325	33.541	39.561	1.00	26.75
ATOM	177	CB	TYR	A	22	67.847	36.225	39.676	1.00	28.34
ATOM	178	CG	TYR	A	22	66.437	35.946	40.154	1.00	30.64
ATOM	179	CD1	TYR	A	22	65.983	36.448	41.367	1.00	31.96
ATOM	180	CD2	TYR	A	22	65.562	35.230	39.361	1.00	32.31
ATOM	181	CE1	TYR	A	22	64.671	36.214	41.795	1.00	32.16
ATOM	182	CE2	TYR	A	22	64.261	34.978	39.779	1.00	32.82
ATOM	183	CZ	TYR	A	22	63.820	35.486	40.987	1.00	36.63
ATOM	184	OH	TYR	A	22	62.518	35.229	41.408	1.00	38.85
ATOM	185	N	GLU	A	23	68.550	33.606	41.669	1.00	34.58
ATOM	186	CA	GLU	A	23	68.528	32.182	41.739	1.00	37.52
ATOM	187	C	GLU	A	23	67.204	31.479	41.529	1.00	42.30
ATOM	188	O	GLU	A	23	67.151	30.280	41.645	1.00	40.71
ATOM	189	CB	GLU	A	23	69.228	31.682	43.000	1.00	39.74
ATOM	190	CG	GLU	A	23	70.712	32.011	43.019	1.00	50.28
ATOM	191	CD	GLU	A	23	71.564	30.874	42.477	1.00	61.64
ATOM	192	OE1	GLU	A	23	71.007	29.955	41.832	1.00	62.40
ATOM	193	OE2	GLU	A	23	72.796	30.894	42.709	1.00	61.54
ATOM	194	N	GLY	A	24	66.124	32.210	41.224	1.00	39.86
ATOM	195	CA	GLY	A	24	64.810	31.560	41.008	1.00	43.77
ATOM	196	C	GLY	A	24	64.377	31.624	39.535	1.00	49.67
ATOM	197	O	GLY	A	24	63.254	31.166	39.188	1.00	54.64
ATOM	198	OH	GLY	A	24	65.142	32.147	38.706	1.00	73.31
ATOM	199	C	PVL	A	25	62.860	38.226	34.454	1.00	17.73

ATOM	200	O	PVL	A	25	63.759	39.046	34.586	1.00	21.35
ATOM	201	CA	PVL	A	25	63.200	36.796	34.251	1.00	26.99
ATOM	202	CB	PVL	A	25	62.057	35.810	34.157	1.00	26.50
ATOM	203	ON	PVL	A	25	64.375	36.432	34.017	1.00	32.90
ATOM	204	N	CYS	A	26	61.544	38.621	34.583	1.00	13.65
ATOM	205	CA	CYS	A	26	61.178	39.997	34.916	1.00	13.69
ATOM	206	CB	CYS	A	26	60.770	40.866	33.674	1.00	19.50
ATOM	207	SG	CYS	A	26	60.527	42.598	34.108	1.00	17.42
ATOM	208	C	CYS	A	26	60.046	39.977	35.926	1.00	17.14
ATOM	209	O	CYS	A	26	58.943	39.511	35.648	1.00	16.98
ATOM	210	N	ALA	A	27	60.356	40.411	37.200	1.00	14.97
ATOM	211	CA	ALA	A	27	59.366	40.425	38.264	1.00	14.51
ATOM	212	C	ALA	A	27	58.675	41.765	38.202	1.00	11.29
ATOM	213	O	ALA	A	27	59.305	42.828	38.099	1.00	13.77
ATOM	214	CB	ALA	A	27	60.106	40.243	39.609	1.00	14.33
ATOM	215	N	ILE	A	28	57.353	41.694	38.222	1.00	12.96
ATOM	216	CA	ILE	A	28	56.491	42.816	38.054	1.00	12.54
ATOM	217	C	ILE	A	28	55.302	42.854	39.067	1.00	13.11
ATOM	218	O	ILE	A	28	54.648	41.858	39.298	1.00	14.34
ATOM	219	CB	ILE	A	28	55.815	42.718	36.559	1.00	13.91
ATOM	220	CG1	ILE	A	28	56.920	42.696	35.525	1.00	15.23
ATOM	221	CG2	ILE	A	28	54.794	43.867	36.283	1.00	16.36
ATOM	222	CD1	ILE	A	28	56.376	42.100	34.149	1.00	17.00
ATOM	223	N	ASP	A	29	55.127	44.025	39.651	1.00	15.10
ATOM	224	CA	ASP	A	29	54.022	44.252	40.636	1.00	14.57
ATOM	225	C	ASP	A	29	52.732	43.607	40.074	1.00	17.57
ATOM	226	O	ASP	A	29	52.315	43.902	38.916	1.00	15.63
ATOM	227	CB	ASP	A	29	53.864	45.728	40.818	1.00	14.77
ATOM	228	CG	ASP	A	29	52.748	46.139	41.788	1.00	14.70
ATOM	229	OD1	ASP	A	29	51.750	45.420	41.984	1.00	15.75
ATOM	230	OD2	ASP	A	29	52.843	47.278	42.239	1.00	16.77
ATOM	231	N	GLN	A	30	52.123	42.710	40.841	1.00	15.71
ATOM	232	CA	GLN	A	30	50.878	42.040	40.414	1.00	16.19
ATOM	233	C	GLN	A	30	49.797	43.037	39.938	1.00	17.73
ATOM	234	O	GLN	A	30	48.961	42.704	39.057	1.00	17.08
ATOM	235	CB	GLN	A	30	50.256	41.249	41.594	1.00	17.85
ATOM	236	CG	GLN	A	30	49.002	40.506	41.200	1.00	23.42
ATOM	237	CD	GLN	A	30	49.272	39.438	40.148	1.00	23.06
ATOM	238	OE1	GLN	A	30	50.062	38.487	40.361	1.00	21.11
ATOM	239	NE2	GLN	A	30	48.588	39.584	38.958	1.00	20.59
ATOM	240	N	ASP	A	31	49.716	44.238	40.516	1.00	16.44
ATOM	241	CA	ASP	A	31	48.714	45.223	40.100	1.00	16.57
ATOM	242	C	ASP	A	31	48.977	45.579	38.606	1.00	17.31
ATOM	243	O	ASP	A	31	47.995	45.769	37.843	1.00	17.32
ATOM	244	CB	ASP	A	31	48.805	46.539	40.892	1.00	19.02
ATOM	245	CG	ASP	A	31	48.138	46.456	42.294	1.00	24.47
ATOM	246	OD1	ASP	A	31	47.188	45.655	42.488	1.00	24.53
ATOM	247	OD2	ASP	A	31	48.596	47.257	43.166	1.00	22.76
ATOM	248	N	PHE	A	32	50.254	45.715	38.254	1.00	14.02
ATOM	249	CA	PHE	A	32	50.643	46.073	36.861	1.00	13.65
ATOM	250	C	PHE	A	32	50.244	44.926	35.950	1.00	16.12
ATOM	251	O	PHE	A	32	49.661	45.197	34.838	1.00	14.39
ATOM	252	CB	PHE	A	32	52.130	46.329	36.726	1.00	13.80
ATOM	253	CG	PHE	A	32	52.665	47.491	37.522	1.00	14.18
ATOM	254	CD1	PHE	A	32	51.860	48.378	38.248	1.00	15.47
ATOM	255	CD2	PHE	A	32	54.035	47.687	37.517	1.00	15.29
ATOM	256	CE1	PHE	A	32	52.485	49.495	38.988	1.00	16.12
ATOM	257	CE2	PHE	A	32	54.634	48.727	38.238	1.00	16.29
ATOM	258	CZ	PHE	A	32	53.855	49.634	38.963	1.00	15.53
ATOM	259	N	LEU	A	33	50.530	43.696	36.347	1.00	15.49

ATOM	260	CA	LEU	A	33	50.165	42.499	35.561	1.00	13.34
ATOM	261	C	LEU	A	33	48.648	42.564	35.331	1.00	17.57
ATOM	262	O	LEU	A	33	48.144	42.392	34.195	1.00	16.65
ATOM	263	CB	LEU	A	33	50.522	41.184	36.282	1.00	14.40
ATOM	264	CG	LEU	A	33	52.018	40.976	36.508	1.00	17.89
ATOM	265	CD1	LEU	A	33	52.222	39.608	37.204	1.00	15.16
ATOM	266	CD2	LEU	A	33	52.716	40.953	35.093	1.00	17.59
ATOM	267	N	ASP	A	34	47.856	42.816	36.382	1.00	15.41
ATOM	268	CA	ASP	A	34	46.391	42.861	36.217	1.00	16.06
ATOM	269	C	ASP	A	34	45.967	43.918	35.169	1.00	18.00
ATOM	270	O	ASP	A	34	45.067	43.667	34.353	1.00	18.35
ATOM	271	CB	ASP	A	34	45.717	43.339	37.556	1.00	18.61
ATOM	272	CG	ASP	A	34	45.731	42.290	38.661	1.00	24.34
ATOM	273	OD1	ASP	A	34	46.077	41.121	38.437	1.00	22.17
ATOM	274	OD2	ASP	A	34	45.349	42.715	39.815	1.00	28.71
ATOM	275	N	ALA	A	35	46.538	45.111	35.239	1.00	13.94
ATOM	276	CA	ALA	A	35	46.146	46.214	34.349	1.00	15.72
ATOM	277	C	ALA	A	35	46.430	45.899	32.899	1.00	17.50
ATOM	278	O	ALA	A	35	45.652	46.304	32.003	1.00	18.53
ATOM	279	CB	ALA	A	35	46.816	47.504	34.742	1.00	16.40
ATOM	280	N	ALA	A	36	47.547	45.207	32.677	1.00	13.80
ATOM	281	CA	ALA	A	36	47.926	44.876	31.274	1.00	14.07
ATOM	282	C	ALA	A	36	47.370	43.515	30.855	1.00	16.21
ATOM	283	O	ALA	A	36	47.595	43.085	29.690	1.00	16.15
ATOM	284	CB	ALA	A	36	49.461	44.944	31.064	1.00	14.23
ATOM	285	N	GLY	A	37	46.670	42.809	31.719	1.00	14.27
ATOM	286	CA	GLY	A	37	46.126	41.505	31.411	1.00	12.78
ATOM	287	C	GLY	A	37	47.249	40.412	31.271	1.00	11.55
ATOM	288	O	GLY	A	37	46.960	39.297	30.764	1.00	13.36
ATOM	289	N	ILE	A	38	48.469	40.675	31.788	1.00	13.57
ATOM	290	CA	ILE	A	38	49.602	39.753	31.728	1.00	13.98
ATOM	291	C	ILE	A	38	49.525	38.785	32.878	1.00	16.32
ATOM	292	O	ILE	A	38	49.168	39.208	34.022	1.00	16.77
ATOM	293	CB	ILE	A	38	50.930	40.521	31.729	1.00	15.34
ATOM	294	CG1	ILE	A	38	50.976	41.423	30.470	1.00	14.55
ATOM	295	CG2	ILE	A	38	52.146	39.592	31.688	1.00	15.27
ATOM	296	CD1	ILE	A	38	52.162	42.332	30.393	1.00	19.63
ATOM	297	N	LEU	A	39	49.805	37.537	32.591	1.00	12.96
ATOM	298	CA	LEU	A	39	49.759	36.442	33.598	1.00	11.40
ATOM	299	C	LEU	A	39	51.134	36.053	34.101	1.00	14.26
ATOM	300	O	LEU	A	39	52.138	36.122	33.435	1.00	13.15
ATOM	301	CB	LEU	A	39	49.109	35.177	33.041	1.00	12.16
ATOM	302	CG	LEU	A	39	47.752	35.258	32.327	1.00	13.32
ATOM	303	CD1	LEU	A	39	47.245	33.957	31.795	1.00	13.99
ATOM	304	CD2	LEU	A	39	46.722	35.899	33.344	1.00	17.01
ATOM	305	N	GLU	A	40	51.183	35.619	35.385	1.00	14.46
ATOM	306	CA	GLU	A	40	52.460	35.148	35.863	1.00	15.39
ATOM	307	C	GLU	A	40	52.828	33.894	34.973	1.00	13.93
ATOM	308	O	GLU	A	40	51.988	33.067	34.640	1.00	13.92
ATOM	309	CB	GLU	A	40	52.292	34.646	37.350	1.00	17.33
ATOM	310	CG	GLU	A	40	53.617	34.054	37.878	1.00	22.86
ATOM	311	CD	GLU	A	40	53.773	34.134	39.395	1.00	37.57
ATOM	312	OE1	GLU	A	40	52.744	33.891	40.044	1.00	29.60
ATOM	313	OE2	GLU	A	40	54.908	34.446	39.887	1.00	24.74
ATOM	314	N	ASN	A	41	54.108	33.828	34.623	1.00	12.53
ATOM	315	CA	ASN	A	41	54.739	32.808	33.826	1.00	12.52
ATOM	316	C	ASN	A	41	54.433	33.020	32.318	1.00	13.84
ATOM	317	O	ASN	A	41	54.806	32.130	31.523	1.00	13.31
ATOM	318	CB	ASN	A	41	54.390	31.431	34.223	1.00	14.21
ATOM	319	CG	ASN	A	41	54.886	31.102	35.690	1.00	18.26

ATOM	320	OD1	ASN	A	41	56.030	31.307	36.004	1.00	19.96
ATOM	321	ND2	ASN	A	41	53.970	30.620	36.521	1.00	23.65
ATOM	322	N	GLU	A	42	53.772	34.119	31.971	1.00	12.49
ATOM	323	CA	GLU	A	42	53.479	34.350	30.505	1.00	11.09
ATOM	324	C	GLU	A	42	54.733	34.843	29.866	1.00	12.61
ATOM	325	O	GLU	A	42	55.513	35.612	30.413	1.00	13.32
ATOM	326	CB	GLU	A	42	52.425	35.399	30.378	1.00	11.37
ATOM	327	CG	GLU	A	42	51.952	35.601	28.887	1.00	13.79
ATOM	328	CD	GLU	A	42	50.768	36.534	28.828	1.00	16.86
ATOM	329	OE1	GLU	A	42	50.420	37.221	29.808	1.00	14.48
ATOM	330	OE2	GLU	A	42	50.126	36.672	27.703	1.00	11.57
ATOM	331	N	ALA	A	43	54.906	34.509	28.554	1.00	11.23
ATOM	332	CA	ALA	A	43	56.007	35.047	27.813	1.00	11.52
ATOM	333	C	ALA	A	43	55.751	36.568	27.567	1.00	12.62
ATOM	334	O	ALA	A	43	54.597	37.005	27.290	1.00	11.29
ATOM	335	CB	ALA	A	43	56.006	34.370	26.420	1.00	11.84
ATOM	336	N	ILE	A	44	56.805	37.359	27.702	1.00	10.61
ATOM	337	CA	ILE	A	44	56.733	38.810	27.493	1.00	9.63
ATOM	338	C	ILE	A	44	57.918	39.296	26.651	1.00	11.21
ATOM	339	O	ILE	A	44	59.026	38.712	26.696	1.00	11.77
ATOM	340	CB	ILE	A	44	56.682	39.604	28.857	1.00	11.13
ATOM	341	CG1	ILE	A	44	57.879	39.178	29.734	1.00	12.75
ATOM	342	CG2	ILE	A	44	55.328	39.346	29.486	1.00	11.62
ATOM	343	CD1	ILE	A	44	58.019	40.058	31.041	1.00	16.57
ATOM	344	N	ASP	A	45	57.676	40.362	25.894	1.00	11.18
ATOM	345	CA	ASP	A	45	58.716	40.991	25.140	1.00	10.11
ATOM	346	C	ASP	A	45	59.008	42.359	25.805	1.00	11.65
ATOM	347	O	ASP	A	45	58.063	43.075	26.222	1.00	12.76
ATOM	348	CB	ASP	A	45	58.208	41.256	23.682	1.00	11.49
ATOM	349	CG	ASP	A	45	57.941	39.984	22.954	1.00	12.09
ATOM	350	OD1	ASP	A	45	58.610	38.923	23.143	1.00	13.27
ATOM	351	OD2	ASP	A	45	56.942	40.040	22.120	1.00	16.15
ATOM	352	N	ILE	A	46	60.287	42.698	25.967	1.00	12.45
ATOM	353	CA	ILE	A	46	60.676	43.964	26.617	1.00	11.69
ATOM	354	C	ILE	A	46	61.478	44.752	25.640	1.00	13.15
ATOM	355	O	ILE	A	46	62.482	44.255	25.076	1.00	13.26
ATOM	356	CB	ILE	A	46	61.482	43.643	27.903	1.00	13.14
ATOM	357	CG1	ILE	A	46	60.601	42.768	28.783	1.00	12.28
ATOM	358	CG2	ILE	A	46	61.923	44.987	28.578	1.00	13.37
ATOM	359	CD1	ILE	A	46	61.243	42.613	30.298	1.00	14.34
ATOM	360	N	TRP	A	47	61.006	45.980	25.380	1.00	12.56
ATOM	361	CA	TRP	A	47	61.641	46.875	24.399	1.00	11.59
ATOM	362	C	TRP	A	47	62.178	48.069	25.241	1.00	12.65
ATOM	363	O	TRP	A	47	61.400	48.793	25.849	1.00	13.30
ATOM	364	CB	TRP	A	47	60.568	47.322	23.405	1.00	11.85
ATOM	365	CG	TRP	A	47	59.929	46.134	22.708	1.00	11.21
ATOM	366	CD1	TRP	A	47	60.560	45.005	22.299	1.00	12.57
ATOM	367	CD2	TRP	A	47	58.558	46.012	22.330	1.00	12.14
ATOM	368	NE1	TRP	A	47	59.646	44.145	21.663	1.00	11.88
ATOM	369	CE2	TRP	A	47	58.417	44.748	21.674	1.00	10.79
ATOM	370	CE3	TRP	A	47	57.437	46.819	22.525	1.00	14.11
ATOM	371	CZ2	TRP	A	47	57.169	44.279	21.207	1.00	11.66
ATOM	372	CZ3	TRP	A	47	56.173	46.361	22.020	1.00	14.28
ATOM	373	CH2	TRP	A	47	56.091	45.074	21.376	1.00	14.15
ATOM	374	N	ASN	A	48	63.480	48.235	25.209	1.00	12.67
ATOM	375	CA	ASN	A	48	64.154	49.253	26.002	1.00	14.84
ATOM	376	C	ASN	A	48	64.201	50.575	25.283	1.00	14.53
ATOM	377	O	ASN	A	48	65.004	50.755	24.291	1.00	15.46
ATOM	378	CB	ASN	A	48	65.526	48.733	26.416	1.00	13.17
ATOM	379	CG	ASN	A	48	66.157	49.544	27.555	1.00	12.09

ATOM	380	OD1	ASN	A	48	66.120	50.736	27.534	1.00	14.55
ATOM	381	ND2	ASN	A	48	66.861	48.842	28.433	1.00	14.53
ATOM	382	N	VAL	A	49	63.389	51.514	25.726	1.00	13.24
ATOM	383	CA	VAL	A	49	63.372	52.806	25.119	1.00	13.19
ATOM	384	C	VAL	A	49	64.680	53.581	25.322	1.00	18.14
ATOM	385	O	VAL	A	49	65.121	54.385	24.480	1.00	19.15
ATOM	386	CB	VAL	A	49	62.180	53.670	25.631	1.00	15.64
ATOM	387	CG1	VAL	A	49	62.151	55.015	24.907	1.00	17.34
ATOM	388	CG2	VAL	A	49	60.838	52.930	25.473	1.00	15.21
ATOM	389	N	THR	A	50	65.328	53.372	26.474	1.00	14.80
ATOM	390	CA	THR	A	50	66.553	54.086	26.727	1.00	14.70
ATOM	391	C	THR	A	50	67.756	53.642	25.869	1.00	15.83
ATOM	392	O	THR	A	50	68.460	54.508	25.322	1.00	18.87
ATOM	393	CB	THR	A	50	66.910	53.985	28.265	1.00	18.21
ATOM	394	OG1	THR	A	50	65.832	54.538	28.996	1.00	15.78
ATOM	395	CG2	THR	A	50	68.159	54.773	28.550	1.00	16.82
ATOM	396	N	ASN	A	51	67.997	52.351	25.772	1.00	14.06
ATOM	397	CA	ASN	A	51	69.160	51.861	25.010	1.00	15.31
ATOM	398	C	ASN	A	51	68.884	51.123	23.688	1.00	17.85
ATOM	399	O	ASN	A	51	69.816	50.692	23.031	1.00	17.40
ATOM	400	CB	ASN	A	51	70.089	51.021	25.909	1.00	18.14
ATOM	401	CG	ASN	A	51	69.476	49.674	26.309	1.00	20.44
ATOM	402	OD1	ASN	A	51	68.497	49.227	25.701	1.00	16.68
ATOM	403	ND2	ASN	A	51	70.059	48.998	27.332	1.00	16.78
ATOM	404	N	GLY	A	52	67.609	50.981	23.350	1.00	15.39
ATOM	405	CA	GLY	A	52	67.235	50.290	22.093	1.00	16.35
ATOM	406	C	GLY	A	52	67.255	48.776	22.108	1.00	18.04
ATOM	407	O	GLY	A	52	66.818	48.153	21.106	1.00	15.14
ATOM	408	N	LYS	A	53	67.728	48.111	23.180	1.00	13.62
ATOM	409	CA	LYS	A	53	67.752	46.655	23.215	1.00	13.33
ATOM	410	C	LYS	A	53	66.349	46.078	23.261	1.00	13.70
ATOM	411	O	LYS	A	53	65.429	46.699	23.798	1.00	13.57
ATOM	412	CB	LYS	A	53	68.618	46.094	24.379	1.00	15.27
ATOM	413	CG	LYS	A	53	70.012	46.653	24.326	1.00	16.18
ATOM	414	CD	LYS	A	53	70.885	45.950	25.341	1.00	18.83
ATOM	415	CE	LYS	A	53	72.239	46.673	25.454	1.00	24.88
ATOM	416	NZ	LYS	A	53	73.095	46.121	26.635	1.00	24.28
ATOM	417	N	ARG	A	54	66.162	44.891	22.656	1.00	12.69
ATOM	418	CA	ARG	A	54	64.873	44.207	22.584	1.00	11.88
ATOM	419	C	ARG	A	54	65.109	42.735	22.949	1.00	14.37
ATOM	420	O	ARG	A	54	65.984	42.067	22.418	1.00	13.79
ATOM	421	CB	ARG	A	54	64.308	44.294	21.128	1.00	11.58
ATOM	422	CG	ARG	A	54	64.188	45.704	20.705	1.00	12.91
ATOM	423	CD	ARG	A	54	63.609	45.807	19.209	1.00	13.98
ATOM	424	NE	ARG	A	54	62.173	45.652	19.138	1.00	15.65
ATOM	425	CZ	ARG	A	54	61.300	46.628	19.354	1.00	13.20
ATOM	426	NH1	ARG	A	54	61.742	47.863	19.705	1.00	13.97
ATOM	427	NH2	ARG	A	54	59.988	46.434	19.232	1.00	12.47
ATOM	428	N	PHE	A	55	64.333	42.196	23.889	1.00	13.21
ATOM	429	CA	PHE	A	55	64.532	40.807	24.304	1.00	11.72
ATOM	430	C	PHE	A	55	63.205	40.203	24.780	1.00	12.09
ATOM	431	O	PHE	A	55	62.219	40.972	25.049	1.00	14.53
ATOM	432	CB	PHE	A	55	65.612	40.693	25.418	1.00	12.81
ATOM	433	CG	PHE	A	55	65.290	41.475	26.699	1.00	14.26
ATOM	434	CD1	PHE	A	55	65.511	42.830	26.778	1.00	15.91
ATOM	435	CD2	PHE	A	55	64.851	40.799	27.810	1.00	16.89
ATOM	436	CE1	PHE	A	55	65.256	43.541	27.972	1.00	18.73
ATOM	437	CE2	PHE	A	55	64.603	41.504	28.989	1.00	18.14
ATOM	438	CZ	PHE	A	55	64.803	42.824	29.062	1.00	16.81
ATOM	439	N	SER	A	56	63.195	38.884	24.887	1.00	12.30

ATOM	440	CA	SER	A	56	62.000	38.137	25.279	1.00	11.60
ATOM	441	C	SER	A	56	62.321	37.267	26.506	1.00	13.08
ATOM	442	O	SER	A	56	63.361	36.664	26.570	1.00	12.92
ATOM	443	CB	SER	A	56	61.485	37.268	24.140	1.00	14.04
ATOM	444	OG	SER	A	56	61.166	38.129	23.026	1.00	17.74
ATOM	445	N	THR	A	57	61.408	37.272	27.461	1.00	12.51
ATOM	446	CA	THR	A	57	61.598	36.500	28.703	1.00	15.14
ATOM	447	C	THR	A	57	60.206	36.070	29.208	1.00	16.57
ATOM	448	O	THR	A	57	59.313	35.793	28.389	1.00	13.36
ATOM	449	CB	THR	A	57	62.368	37.331	29.719	1.00	17.35
ATOM	450	OG1	THR	A	57	62.652	36.502	30.862	1.00	17.51
ATOM	451	CG2	THR	A	57	61.695	38.645	30.120	1.00	19.79
ATOM	452	N	TYR	A	58	59.971	35.950	30.539	1.00	13.07
ATOM	453	CA	TYR	A	58	58.641	35.565	31.042	1.00	11.86
ATOM	454	C	TYR	A	58	58.405	36.396	32.333	1.00	14.46
ATOM	455	O	TYR	A	58	59.351	36.898	32.907	1.00	14.80
ATOM	456	CB	TYR	A	58	58.474	34.094	31.314	1.00	11.64
ATOM	457	CG	TYR	A	58	59.412	33.543	32.372	1.00	14.08
ATOM	458	CD1	TYR	A	58	60.722	33.204	32.057	1.00	14.47
ATOM	459	CD2	TYR	A	58	58.962	33.402	33.703	1.00	16.79
ATOM	460	CE1	TYR	A	58	61.591	32.711	33.019	1.00	19.79
ATOM	461	CE2	TYR	A	58	59.850	32.890	34.685	1.00	15.79
ATOM	462	CZ	TYR	A	58	61.134	32.569	34.321	1.00	22.24
ATOM	463	OH	TYR	A	58	61.935	32.108	35.380	1.00	23.11
ATOM	464	N	ALA	A	59	57.139	36.566	32.673	1.00	11.72
ATOM	465	CA	ALA	A	59	56.764	37.373	33.834	1.00	12.72
ATOM	466	C	ALA	A	59	56.719	36.582	35.105	1.00	12.49
ATOM	467	O	ALA	A	59	56.191	35.479	35.157	1.00	13.37
ATOM	468	CB	ALA	A	59	55.325	37.956	33.607	1.00	13.81
ATOM	469	N	ILE	A	60	57.259	37.249	36.146	1.00	15.14
ATOM	470	CA	ILE	A	60	57.221	36.693	37.546	1.00	16.33
ATOM	471	C	ILE	A	60	56.402	37.733	38.349	1.00	16.77
ATOM	472	O	ILE	A	60	56.575	38.937	38.182	1.00	14.68
ATOM	473	CB	ILE	A	60	58.619	36.674	38.126	1.00	18.30
ATOM	474	CG1	ILE	A	60	59.497	35.633	37.421	1.00	19.09
ATOM	475	CG2	ILE	A	60	58.553	36.414	39.697	1.00	21.06
ATOM	476	CD1	ILE	A	60	60.986	35.801	37.681	1.00	26.31
ATOM	477	N	ALA	A	61	55.480	37.268	39.208	1.00	15.66
ATOM	478	CA	ALA	A	61	54.713	38.264	39.966	1.00	15.73
ATOM	479	C	ALA	A	61	55.517	38.764	41.199	1.00	18.47
ATOM	480	O	ALA	A	61	56.163	37.978	41.882	1.00	23.19
ATOM	481	CB	ALA	A	61	53.384	37.696	40.428	1.00	17.99
ATOM	482	N	ALA	A	62	55.470	40.063	41.393	1.00	14.95
ATOM	483	CA	ALA	A	62	56.093	40.757	42.560	1.00	14.55
ATOM	484	C	ALA	A	62	54.872	41.146	43.391	1.00	18.92
ATOM	485	O	ALA	A	62	53.715	41.217	42.964	1.00	17.86
ATOM	486	CB	ALA	A	62	56.883	42.004	42.189	1.00	13.98
ATOM	487	N	GLU	A	63	55.159	41.391	44.690	1.00	17.78
ATOM	488	CA	GLU	A	63	54.108	41.762	45.620	1.00	19.52
ATOM	489	C	GLU	A	63	53.226	42.917	45.151	1.00	19.81
ATOM	490	O	GLU	A	63	53.728	43.915	44.654	1.00	17.13
ATOM	491	CB	GLU	A	63	54.809	42.221	46.926	1.00	21.37
ATOM	492	CG	GLU	A	63	53.838	42.563	48.082	1.00	29.86
ATOM	493	CD	GLU	A	63	54.387	43.633	49.041	1.00	53.22
ATOM	494	OE1	GLU	A	63	55.572	44.035	48.935	1.00	44.04
ATOM	495	OE2	GLU	A	63	53.610	44.064	49.915	1.00	43.79
ATOM	496	N	ARG	A	64	51.924	42.783	45.347	1.00	16.26
ATOM	497	CA	ARG	A	64	50.979	43.805	44.987	1.00	16.34
ATOM	498	C	ARG	A	64	51.297	45.121	45.697	1.00	21.13
ATOM	499	O	ARG	A	64	51.433	45.142	46.954	1.00	20.36

ATOM	500	CB	ARG	A	64	49.552	43.360	45.289	1.00	19.26
ATOM	501	CG	ARG	A	64	48.544	44.299	44.749	1.00	26.38
ATOM	502	CD	ARG	A	64	47.108	43.842	44.982	1.00	27.64
ATOM	503	NE	ARG	A	64	46.789	42.467	44.605	1.00	26.53
ATOM	504	CZ	ARG	A	64	46.420	42.092	43.371	1.00	41.54
ATOM	505	NH1	ARG	A	64	46.373	42.981	42.364	1.00	23.51
ATOM	506	NH2	ARG	A	64	46.122	40.831	43.137	1.00	30.75
ATOM	507	N	GLY	A	65	51.430	46.204	44.963	1.00	17.09
ATOM	508	CA	GLY	A	65	51.707	47.513	45.507	1.00	17.60
ATOM	509	C	GLY	A	65	53.195	47.853	45.639	1.00	18.83
ATOM	510	O	GLY	A	65	53.551	48.980	46.004	1.00	20.21
ATOM	511	N	SER	A	66	54.074	46.897	45.329	1.00	16.18
ATOM	512	CA	SER	A	66	55.502	47.099	45.413	1.00	15.57
ATOM	513	C	SER	A	66	56.089	47.993	44.302	1.00	19.13
ATOM	514	O	SER	A	66	57.144	48.615	44.440	1.00	18.34
ATOM	515	CB	SER	A	66	56.223	45.788	45.382	1.00	18.61
ATOM	516	OG	SER	A	66	56.092	45.139	44.066	1.00	17.83
ATOM	517	N	ARG	A	67	55.339	48.040	43.176	1.00	16.53
ATOM	518	CA	ARG	A	67	55.762	48.826	41.973	1.00	17.76
ATOM	519	C	ARG	A	67	57.111	48.346	41.419	1.00	14.93
ATOM	520	O	ARG	A	67	57.803	49.101	40.784	1.00	16.56
ATOM	521	CB	ARG	A	67	55.791	50.324	42.242	1.00	15.58
ATOM	522	CG	ARG	A	67	54.431	50.904	42.651	1.00	14.91
ATOM	523	CD	ARG	A	67	54.376	52.362	42.553	1.00	13.81
ATOM	524	NE	ARG	A	67	53.069	52.872	43.035	1.00	16.78
ATOM	525	CZ	ARG	A	67	52.677	54.135	42.909	1.00	18.26
ATOM	526	NH1	ARG	A	67	53.438	55.053	42.332	1.00	18.16
ATOM	527	NH2	ARG	A	67	51.487	54.504	43.395	1.00	19.31
ATOM	528	N	ILE	A	68	57.444	47.091	41.670	1.00	13.92
ATOM	529	CA	ILE	A	68	58.720	46.535	41.233	1.00	13.11
ATOM	530	C	ILE	A	68	58.661	46.183	39.704	1.00	14.96
ATOM	531	O	ILE	A	68	57.632	45.692	39.216	1.00	16.08
ATOM	532	CB	ILE	A	68	59.009	45.237	42.014	1.00	16.07
ATOM	533	CG1	ILE	A	68	59.387	45.593	43.529	1.00	15.43
ATOM	534	CG2	ILE	A	68	60.143	44.394	41.325	1.00	14.91
ATOM	535	CD1	ILE	A	68	59.427	44.398	44.371	1.00	17.12
ATOM	536	N	ILE	A	69	59.782	46.449	39.064	1.00	15.79
ATOM	537	CA	ILE	A	69	60.095	46.043	37.673	1.00	14.43
ATOM	538	C	ILE	A	69	61.570	45.598	37.885	1.00	12.91
ATOM	539	O	ILE	A	69	62.494	46.446	37.839	1.00	16.10
ATOM	540	CB	ILE	A	69	60.003	47.141	36.653	1.00	14.38
ATOM	541	CG1	ILE	A	69	58.579	47.740	36.528	1.00	14.18
ATOM	542	CG2	ILE	A	69	60.415	46.555	35.241	1.00	14.77
ATOM	543	CD1	ILE	A	69	57.484	46.764	35.993	1.00	13.25
ATOM	544	N	SER	A	70	61.794	44.306	38.101	1.00	12.61
ATOM	545	CA	SER	A	70	63.124	43.778	38.331	1.00	12.79
ATOM	546	C	SER	A	70	63.559	42.861	37.151	1.00	16.65
ATOM	547	O	SER	A	70	62.929	41.846	36.887	1.00	16.44
ATOM	548	CB	SER	A	70	63.136	42.977	39.663	1.00	17.19
ATOM	549	OG	SER	A	70	64.479	42.512	39.964	1.00	19.28
ATOM	550	N	VAL	A	71	64.653	43.229	36.521	1.00	16.77
ATOM	551	CA	VAL	A	71	65.194	42.443	35.375	1.00	16.54
ATOM	552	C	VAL	A	71	66.231	41.490	36.002	1.00	18.47
ATOM	553	O	VAL	A	71	67.253	41.930	36.571	1.00	20.32
ATOM	554	CB	VAL	A	71	65.746	43.437	34.301	1.00	21.34
ATOM	555	CG1	VAL	A	71	66.394	42.692	33.158	1.00	23.85
ATOM	556	CG2	VAL	A	71	64.618	44.286	33.711	1.00	21.90
ATOM	557	N	ASN	A	72	65.953	40.204	35.942	1.00	17.21
ATOM	558	CA	ASN	A	72	66.764	39.178	36.560	1.00	18.06
ATOM	559	C	ASN	A	72	67.441	38.224	35.601	1.00	22.03

ATOM	560	O	ASN	A	72	67.039	38.141	34.422	1.00	20.77
ATOM	561	CB	ASN	A	72	65.847	38.323	37.470	1.00	15.71
ATOM	562	CG	ASN	A	72	65.116	39.170	38.557	1.00	21.14
ATOM	563	OD1	ASN	A	72	65.574	40.229	38.928	1.00	22.76
ATOM	564	ND2	ASN	A	72	63.951	38.678	38.978	1.00	26.84
ATOM	565	N	GLY	A	73	68.433	37.487	36.082	1.00	17.96
ATOM	566	CA	GLY	A	73	69.132	36.519	35.239	1.00	17.13
ATOM	567	C	GLY	A	73	69.886	37.193	34.124	1.00	17.10
ATOM	568	O	GLY	A	73	70.357	38.314	34.238	1.00	17.56
ATOM	569	N	ALA	A	74	69.996	36.475	33.003	1.00	16.81
ATOM	570	CA	ALA	A	74	70.743	37.040	31.860	1.00	16.63
ATOM	571	C	ALA	A	74	70.172	38.361	31.377	1.00	17.98
ATOM	572	O	ALA	A	74	70.911	39.200	30.838	1.00	17.87
ATOM	573	CB	ALA	A	74	70.760	36.034	30.703	1.00	16.76
ATOM	574	N	ALA	A	75	68.859	38.568	31.576	1.00	16.77
ATOM	575	CA	ALA	A	75	68.214	39.834	31.160	1.00	17.69
ATOM	576	C	ALA	A	75	68.855	41.099	31.787	1.00	17.68
ATOM	577	O	ALA	A	75	68.716	42.194	31.279	1.00	16.79
ATOM	578	CB	ALA	A	75	66.761	39.816	31.504	1.00	20.55
ATOM	579	N	ALA	A	76	69.556	40.921	32.930	1.00	16.67
ATOM	580	CA	ALA	A	76	70.183	42.082	33.556	1.00	17.52
ATOM	581	C	ALA	A	76	71.296	42.721	32.665	1.00	17.22
ATOM	582	O	ALA	A	76	71.738	43.846	32.900	1.00	18.09
ATOM	583	CB	ALA	A	76	70.695	41.726	34.989	1.00	18.29
ATOM	584	N	HIS	A	77	71.713	42.004	31.593	1.00	15.19
ATOM	585	CA	HIS	A	77	72.705	42.553	30.666	1.00	16.72
ATOM	586	C	HIS	A	77	71.996	43.452	29.623	1.00	16.17
ATOM	587	O	HIS	A	77	72.681	44.164	28.872	1.00	18.25
ATOM	588	CB	HIS	A	77	73.300	41.399	29.823	1.00	18.31
ATOM	589	CG	HIS	A	77	74.342	40.606	30.525	1.00	21.21
ATOM	590	ND1	HIS	A	77	75.625	41.057	30.668	1.00	25.21
ATOM	591	CD2	HIS	A	77	74.303	39.384	31.099	1.00	22.31
ATOM	592	CE1	HIS	A	77	76.336	40.153	31.323	1.00	23.74
ATOM	593	NE2	HIS	A	77	75.564	39.124	31.586	1.00	22.33
ATOM	594	N	CYS	A	78	70.666	43.404	29.585	1.00	14.86
ATOM	595	CA	CYS	A	78	69.896	44.162	28.587	1.00	16.42
ATOM	596	C	CYS	A	78	69.145	45.376	29.085	1.00	16.96
ATOM	597	O	CYS	A	78	68.579	46.190	28.270	1.00	16.97
ATOM	598	CB	CYS	A	78	68.863	43.235	27.909	1.00	16.76
ATOM	599	SG	CYS	A	78	69.588	41.704	27.164	1.00	22.74
ATOM	600	N	ALA	A	79	69.075	45.549	30.440	1.00	14.78
ATOM	601	CA	ALA	A	79	68.366	46.701	30.991	1.00	14.85
ATOM	602	C	ALA	A	79	69.025	46.988	32.351	1.00	15.30
ATOM	603	O	ALA	A	79	69.567	46.065	32.964	1.00	16.51
ATOM	604	CB	ALA	A	79	66.885	46.431	31.178	1.00	15.77
ATOM	605	N	SER	A	80	68.971	48.263	32.704	1.00	13.90
ATOM	606	CA	SER	A	80	69.558	48.764	33.982	1.00	13.46
ATOM	607	C	SER	A	80	68.547	49.548	34.747	1.00	17.54
ATOM	608	O	SER	A	80	67.589	50.071	34.213	1.00	16.85
ATOM	609	CB	SER	A	80	70.739	49.652	33.656	1.00	17.79
ATOM	610	OG	SER	A	80	71.725	48.905	32.934	1.00	18.84
ATOM	611	N	VAL	A	81	68.788	49.664	36.076	1.00	15.99
ATOM	612	CA	VAL	A	81	67.897	50.448	36.907	1.00	14.74
ATOM	613	C	VAL	A	81	67.879	51.877	36.357	1.00	14.78
ATOM	614	O	VAL	A	81	68.899	52.500	36.103	1.00	15.81
ATOM	615	CB	VAL	A	81	68.468	50.470	38.409	1.00	14.01
ATOM	616	CG1	VAL	A	81	67.606	51.444	39.242	1.00	15.95
ATOM	617	CG2	VAL	A	81	68.363	49.104	39.020	1.00	15.67
ATOM	618	N	GLY	A	82	66.689	52.420	36.132	1.00	14.65
ATOM	619	CA	GLY	A	82	66.551	53.734	35.586	1.00	14.30

ATOM	620	C	GLY	A	82	66.072	53.721	34.113	1.00	16.91
ATOM	621	O	GLY	A	82	65.494	54.699	33.664	1.00	15.50
ATOM	622	N	ASP	A	83	66.347	52.624	33.431	1.00	14.93
ATOM	623	CA	ASP	A	83	65.911	52.551	31.994	1.00	13.74
ATOM	624	C	ASP	A	83	64.391	52.545	31.907	1.00	14.63
ATOM	625	O	ASP	A	83	63.687	51.980	32.775	1.00	15.91
ATOM	626	CB	ASP	A	83	66.421	51.242	31.319	1.00	13.28
ATOM	627	CG	ASP	A	83	67.917	51.248	31.004	1.00	12.11
ATOM	628	OD1	ASP	A	83	68.614	52.301	31.107	1.00	15.32
ATOM	629	OD2	ASP	A	83	68.382	50.116	30.667	1.00	15.76
ATOM	630	N	ILE	A	84	63.879	53.153	30.818	1.00	14.29
ATOM	631	CA	ILE	A	84	62.442	53.204	30.547	1.00	13.65
ATOM	632	C	ILE	A	84	62.169	52.078	29.504	1.00	13.60
ATOM	633	O	ILE	A	84	62.896	51.987	28.514	1.00	15.62
ATOM	634	CB	ILE	A	84	62.092	54.551	29.873	1.00	16.83
ATOM	635	CG1	ILE	A	84	62.350	55.760	30.847	1.00	17.52
ATOM	636	CG2	ILE	A	84	60.633	54.554	29.440	1.00	19.25
ATOM	637	CD1	ILE	A	84	61.480	55.706	32.107	1.00	21.07
ATOM	638	N	VAL	A	85	61.212	51.235	29.785	1.00	12.41
ATOM	639	CA	VAL	A	85	60.934	50.112	28.876	1.00	12.94
ATOM	640	C	VAL	A	85	59.475	49.946	28.633	1.00	15.89
ATOM	641	O	VAL	A	85	58.583	50.517	29.317	1.00	14.01
ATOM	642	CB	VAL	A	85	61.466	48.783	29.474	1.00	14.37
ATOM	643	CG1	VAL	A	85	62.960	48.870	29.885	1.00	13.95
ATOM	644	CG2	VAL	A	85	60.649	48.332	30.741	1.00	14.77
ATOM	645	N	ILE	A	86	59.162	49.117	27.608	1.00	13.28
ATOM	646	CA	ILE	A	86	57.778	48.809	27.263	1.00	13.39
ATOM	647	C	ILE	A	86	57.723	47.283	27.366	1.00	14.02
ATOM	648	O	ILE	A	86	58.586	46.593	26.825	1.00	13.98
ATOM	649	CB	ILE	A	86	57.418	49.286	25.801	1.00	13.99
ATOM	650	CG1	ILE	A	86	57.347	50.842	25.764	1.00	17.59
ATOM	651	CG2	ILE	A	86	56.067	48.669	25.419	1.00	15.22
ATOM	652	CD1	ILE	A	86	57.543	51.448	24.363	1.00	22.03
ATOM	653	N	ILE	A	87	56.779	46.734	28.149	1.00	12.05
ATOM	654	CA	ILE	A	87	56.654	45.304	28.337	1.00	11.27
ATOM	655	C	ILE	A	87	55.336	44.865	27.730	1.00	12.08
ATOM	656	O	ILE	A	87	54.252	45.364	28.075	1.00	13.19
ATOM	657	CB	ILE	A	87	56.693	44.934	29.905	1.00	12.91
ATOM	658	CG1	ILE	A	87	57.972	45.491	30.455	1.00	14.33
ATOM	659	CG2	ILE	A	87	56.572	43.438	30.062	1.00	14.68
ATOM	660	CD1	ILE	A	87	58.085	45.263	32.060	1.00	14.91
ATOM	661	N	ALA	A	88	55.416	43.891	26.782	1.00	11.17
ATOM	662	CA	ALA	A	88	54.209	43.441	26.124	1.00	11.51
ATOM	663	C	ALA	A	88	53.978	41.975	26.112	1.00	11.06
ATOM	664	O	ALA	A	88	54.949	41.191	26.190	1.00	12.85
ATOM	665	CB	ALA	A	88	54.372	43.905	24.582	1.00	12.18
ATOM	666	N	SER	A	89	52.719	41.526	25.953	1.00	11.32
ATOM	667	CA	SER	A	89	52.459	40.087	25.769	1.00	11.17
ATOM	668	C	SER	A	89	51.547	39.992	24.538	1.00	11.44
ATOM	669	O	SER	A	89	50.833	40.964	24.213	1.00	11.04
ATOM	670	CB	SER	A	89	51.858	39.327	26.979	1.00	14.68
ATOM	671	OG	SER	A	89	50.438	39.480	27.037	1.00	13.56
ATOM	672	N	PHE	A	90	51.691	38.849	23.860	1.00	11.58
ATOM	673	CA	PHE	A	90	50.894	38.604	22.632	1.00	10.03
ATOM	674	C	PHE	A	90	50.125	37.331	22.780	1.00	11.41
ATOM	675	O	PHE	A	90	50.615	36.342	23.436	1.00	12.95
ATOM	676	CB	PHE	A	90	51.867	38.480	21.438	1.00	10.86
ATOM	677	CG	PHE	A	90	52.457	39.784	21.010	1.00	11.25
ATOM	678	CD1	PHE	A	90	53.611	40.322	21.617	1.00	12.54
ATOM	679	CD2	PHE	A	90	51.824	40.536	19.976	1.00	13.88

ATOM	680	CE1	PHE	A	90	54.134	41.602	21.173	1.00	12.35
ATOM	681	CE2	PHE	A	90	52.304	41.729	19.539	1.00	13.61
ATOM	682	CZ	PHE	A	90	53.459	42.314	20.114	1.00	12.98
ATOM	683	N	VAL	A	91	48.928	37.303	22.178	1.00	9.83
ATOM	684	CA	VAL	A	91	48.073	36.118	22.213	1.00	10.22
ATOM	685	C	VAL	A	91	47.588	35.798	20.793	1.00	14.03
ATOM	686	O	VAL	A	91	47.690	36.675	19.893	1.00	13.50
ATOM	687	CB	VAL	A	91	46.803	36.261	23.098	1.00	13.62
ATOM	688	CG1	VAL	A	91	47.217	36.266	24.596	1.00	15.08
ATOM	689	CG2	VAL	A	91	45.999	37.507	22.722	1.00	13.05
ATOM	690	N	THR	A	92	47.154	34.586	20.611	1.00	12.76
ATOM	691	CA	THR	A	92	46.628	34.182	19.275	1.00	11.56
ATOM	692	C	THR	A	92	45.132	33.971	19.349	1.00	13.31
ATOM	693	O	THR	A	92	44.530	33.582	20.391	1.00	13.08
ATOM	694	CB	THR	A	92	47.340	32.987	18.626	1.00	12.64
ATOM	695	OG1	THR	A	92	47.132	31.797	19.427	1.00	16.06
ATOM	696	CG2	THR	A	92	48.849	33.212	18.472	1.00	13.80
ATOM	697	N	MET	A	93	44.412	34.267	18.224	1.00	11.69
ATOM	698	CA	MET	A	93	42.951	34.108	18.147	1.00	11.35
ATOM	699	C	MET	A	93	42.609	34.143	16.641	1.00	14.45
ATOM	700	O	MET	A	93	43.429	34.572	15.835	1.00	13.44
ATOM	701	CB	MET	A	93	42.224	35.317	18.831	1.00	12.85
ATOM	702	CG	MET	A	93	42.628	36.660	18.178	1.00	13.91
ATOM	703	SD	MET	A	93	42.084	38.126	19.099	1.00	14.46
ATOM	704	CE	MET	A	93	43.261	37.982	20.500	1.00	14.10
ATOM	705	N	PRO	A	94	41.440	33.664	16.331	1.00	12.36
ATOM	706	CA	PRO	A	94	40.994	33.662	14.921	1.00	12.35
ATOM	707	C	PRO	A	94	40.927	35.119	14.384	1.00	15.66
ATOM	708	O	PRO	A	94	40.708	36.116	15.069	1.00	14.35
ATOM	709	CB	PRO	A	94	39.592	33.150	15.005	1.00	13.86
ATOM	710	CG	PRO	A	94	39.606	32.186	16.204	1.00	15.72
ATOM	711	CD	PRO	A	94	40.405	33.060	17.191	1.00	12.82
ATOM	712	N	ASP	A	95	41.040	35.223	13.035	1.00	14.03
ATOM	713	CA	ASP	A	95	40.966	36.538	12.434	1.00	15.39
ATOM	714	C	ASP	A	95	39.760	37.423	12.789	1.00	16.06
ATOM	715	O	ASP	A	95	39.886	38.651	12.959	1.00	16.29
ATOM	716	CB	ASP	A	95	40.998	36.355	10.903	1.00	15.44
ATOM	717	CG	ASP	A	95	41.147	37.685	10.168	1.00	15.85
ATOM	718	OD1	ASP	A	95	42.199	38.354	10.289	1.00	14.33
ATOM	719	OD2	ASP	A	95	40.178	38.088	9.441	1.00	18.70
ATOM	720	N	GLU	A	96	38.571	36.831	12.864	1.00	15.70
ATOM	721	CA	GLU	A	96	37.389	37.631	13.182	1.00	14.32
ATOM	722	C	GLU	A	96	37.468	38.304	14.550	1.00	18.35
ATOM	723	O	GLU	A	96	37.196	39.487	14.686	1.00	17.78
ATOM	724	CB	GLU	A	96	36.102	36.828	12.995	1.00	16.31
ATOM	725	CG	GLU	A	96	34.860	37.623	13.365	1.00	22.63
ATOM	726	CD	GLU	A	96	33.526	36.880	13.068	1.00	23.98
ATOM	727	OE1	GLU	A	96	33.559	35.704	12.706	1.00	25.84
ATOM	728	OE2	GLU	A	96	32.461	37.497	13.246	1.00	30.53
ATOM	729	N	GLU	A	97	37.863	37.514	15.545	1.00	15.16
ATOM	730	CA	GLU	A	97	37.999	38.111	16.875	1.00	15.52
ATOM	731	C	GLU	A	97	39.128	39.177	16.850	1.00	13.99
ATOM	732	O	GLU	A	97	39.028	40.206	17.493	1.00	16.67
ATOM	733	CB	GLU	A	97	38.338	36.990	17.857	1.00	15.35
ATOM	734	CG	GLU	A	97	38.566	37.525	19.290	1.00	17.59
ATOM	735	CD	GLU	A	97	38.814	36.394	20.261	1.00	22.36
ATOM	736	OE1	GLU	A	97	38.899	35.209	19.850	1.00	17.71
ATOM	737	OE2	GLU	A	97	38.890	36.747	21.481	1.00	22.62
ATOM	738	N	ALA	A	98	40.228	38.917	16.123	1.00	13.03
ATOM	739	CA	ALA	A	98	41.349	39.850	16.036	1.00	12.71

ATOM	740	C	ALA	A	98	40.957	41.219	15.463	1.00	15.63
ATOM	741	O	ALA	A	98	41.496	42.253	15.834	1.00	14.36
ATOM	742	CB	ALA	A	98	42.463	39.223	15.190	1.00	14.85
ATOM	743	N	ARG	A	99	39.959	41.235	14.534	1.00	14.05
ATOM	744	CA	ARG	A	99	39.565	42.490	13.944	1.00	15.96
ATOM	745	C	ARG	A	99	38.883	43.474	14.862	1.00	17.44
ATOM	746	O	ARG	A	99	38.845	44.666	14.535	1.00	21.21
ATOM	747	CB	ARG	A	99	38.743	42.259	12.633	1.00	17.37
ATOM	748	CG	ARG	A	99	39.630	41.725	11.515	1.00	16.32
ATOM	749	CD	ARG	A	99	38.869	41.511	10.154	1.00	16.45
ATOM	750	NE	ARG	A	99	38.150	40.252	10.074	1.00	14.75
ATOM	751	CZ	ARG	A	99	36.851	40.106	10.202	1.00	13.61
ATOM	752	NH1	ARG	A	99	36.084	41.162	10.415	1.00	16.09
ATOM	753	NH2	ARG	A	99	36.306	38.906	10.083	1.00	18.40
ATOM	754	N	THR	A	100	38.364	43.021	15.998	1.00	16.42
ATOM	755	CA	THR	A	100	37.753	43.988	16.917	1.00	16.33
ATOM	756	C	THR	A	100	38.350	43.803	18.317	1.00	19.97
ATOM	757	O	THR	A	100	37.735	44.220	19.329	1.00	20.03
ATOM	758	CB	THR	A	100	36.246	43.908	17.014	1.00	21.91
ATOM	759	OG1	THR	A	100	35.822	42.556	17.266	1.00	20.66
ATOM	760	CG2	THR	A	100	35.626	44.354	15.658	1.00	22.68
ATOM	761	N	TRP	A	101	39.533	43.203	18.349	1.00	17.87
ATOM	762	CA	TRP	A	101	40.199	42.981	19.671	1.00	16.71
ATOM	763	C	TRP	A	101	40.710	44.288	20.258	1.00	19.04
ATOM	764	O	TRP	A	101	41.247	45.135	19.540	1.00	17.05
ATOM	765	CB	TRP	A	101	41.390	42.038	19.455	1.00	14.65
ATOM	766	CG	TRP	A	101	42.311	41.932	20.694	1.00	14.16
ATOM	767	CD1	TRP	A	101	43.528	42.444	20.800	1.00	16.31
ATOM	768	CD2	TRP	A	101	42.034	41.196	21.899	1.00	16.31
ATOM	769	NE1	TRP	A	101	44.070	42.124	22.085	1.00	15.49
ATOM	770	CE2	TRP	A	101	43.151	41.365	22.743	1.00	17.23
ATOM	771	CE3	TRP	A	101	40.944	40.448	22.362	1.00	19.60
ATOM	772	CZ2	TRP	A	101	43.211	40.796	24.037	1.00	18.02
ATOM	773	CZ3	TRP	A	101	41.013	39.854	23.639	1.00	21.23
ATOM	774	CH2	TRP	A	101	42.136	40.045	24.443	1.00	21.41
ATOM	775	N	ARG	A	102	40.563	44.465	21.612	1.00	15.76
ATOM	776	CA	ARG	A	102	41.070	45.703	22.235	1.00	16.64
ATOM	777	C	ARG	A	102	42.180	45.344	23.275	1.00	14.79
ATOM	778	O	ARG	A	102	41.838	44.748	24.316	1.00	17.03
ATOM	779	CB	ARG	A	102	39.943	46.431	22.963	1.00	17.42
ATOM	780	CG	ARG	A	102	38.775	46.821	22.058	1.00	24.67
ATOM	781	CD	ARG	A	102	39.285	47.662	20.922	1.00	40.94
ATOM	782	NE	ARG	A	102	38.215	47.967	19.971	1.00	58.76
ATOM	783	CZ	ARG	A	102	38.246	47.668	18.668	1.00	65.94
ATOM	784	NH1	ARG	A	102	39.307	47.043	18.135	1.00	46.00
ATOM	785	NH2	ARG	A	102	37.211	47.987	17.896	1.00	52.57
ATOM	786	N	PRO	A	103	43.422	45.671	22.999	1.00	15.12
ATOM	787	CA	PRO	A	103	44.515	45.313	23.948	1.00	13.53
ATOM	788	C	PRO	A	103	44.329	46.058	25.274	1.00	15.29
ATOM	789	O	PRO	A	103	43.749	47.117	25.309	1.00	16.02
ATOM	790	CB	PRO	A	103	45.770	45.786	23.270	1.00	14.34
ATOM	791	CG	PRO	A	103	45.386	45.801	21.717	1.00	18.46
ATOM	792	CD	PRO	A	103	43.942	46.250	21.748	1.00	15.59
ATOM	793	N	ASN	A	104	44.884	45.445	26.347	1.00	14.28
ATOM	794	CA	ASN	A	104	44.836	46.034	27.698	1.00	13.04
ATOM	795	C	ASN	A	104	46.119	46.863	27.862	1.00	14.43
ATOM	796	O	ASN	A	104	47.217	46.296	28.125	1.00	13.98
ATOM	797	CB	ASN	A	104	44.760	44.875	28.655	1.00	12.98
ATOM	798	CG	ASN	A	104	43.490	44.121	28.510	1.00	15.09
ATOM	799	OD1	ASN	A	104	42.398	44.706	28.655	1.00	17.92

ATOM	800	ND2	ASN	A	104	43.569	42.842	28.158	1.00	16.93
ATOM	801	N	VAL	A	105	46.019	48.179	27.673	1.00	14.40
ATOM	802	CA	VAL	A	105	47.150	49.048	27.734	1.00	15.19
ATOM	803	C	VAL	A	105	47.164	49.895	28.992	1.00	18.79
ATOM	804	O	VAL	A	105	46.172	50.559	29.309	1.00	20.46
ATOM	805	CB	VAL	A	105	47.188	50.005	26.534	1.00	18.28
ATOM	806	CG1	VAL	A	105	48.423	50.904	26.591	1.00	20.67
ATOM	807	CG2	VAL	A	105	47.223	49.166	25.186	1.00	17.51
ATOM	808	N	ALA	A	106	48.297	49.853	29.683	1.00	16.66
ATOM	809	CA	ALA	A	106	48.457	50.694	30.921	1.00	16.75
ATOM	810	C	ALA	A	106	49.647	51.596	30.665	1.00	15.84
ATOM	811	O	ALA	A	106	50.711	51.115	30.266	1.00	16.27
ATOM	812	CB	ALA	A	106	48.672	49.807	32.141	1.00	17.32
ATOM	813	N	TYR	A	107	49.475	52.911	30.905	1.00	15.99
ATOM	814	CA	TYR	A	107	50.474	53.931	30.697	1.00	15.93
ATOM	815	C	TYR	A	107	51.037	54.390	32.046	1.00	18.71
ATOM	816	O	TYR	A	107	50.287	54.506	33.007	1.00	20.84
ATOM	817	CB	TYR	A	107	49.901	55.154	29.951	1.00	19.26
ATOM	818	CG	TYR	A	107	49.419	54.812	28.533	1.00	21.14
ATOM	819	CD1	TYR	A	107	50.291	54.819	27.490	1.00	21.91
ATOM	820	CD2	TYR	A	107	48.106	54.510	28.307	1.00	23.16
ATOM	821	CE1	TYR	A	107	49.861	54.497	26.190	1.00	24.59
ATOM	822	CE2	TYR	A	107	47.672	54.182	27.007	1.00	24.09
ATOM	823	CZ	TYR	A	107	48.571	54.197	25.992	1.00	27.50
ATOM	824	OH	TYR	A	107	48.200	53.880	24.685	1.00	29.66
ATOM	825	N	PHE	A	108	52.340	54.609	32.042	1.00	15.42
ATOM	826	CA	PHE	A	108	53.049	55.012	33.297	1.00	15.71
ATOM	827	C	PHE	A	108	53.868	56.249	33.162	1.00	19.91
ATOM	828	O	PHE	A	108	54.268	56.703	32.071	1.00	19.12
ATOM	829	CB	PHE	A	108	53.974	53.876	33.723	1.00	16.87
ATOM	830	CG	PHE	A	108	53.258	52.651	34.125	1.00	16.76
ATOM	831	CD1	PHE	A	108	52.842	51.702	33.160	1.00	17.17
ATOM	832	CD2	PHE	A	108	52.940	52.381	35.481	1.00	17.45
ATOM	833	CE1	PHE	A	108	52.147	50.577	33.546	1.00	19.62
ATOM	834	CE2	PHE	A	108	52.242	51.243	35.867	1.00	20.41
ATOM	835	CZ	PHE	A	108	51.838	50.301	34.901	1.00	19.54
ATOM	836	N	GLU	A	109	54.193	56.830	34.342	1.00	17.02
ATOM	837	CA	GLU	A	109	55.053	58.009	34.382	1.00	17.21
ATOM	838	C	GLU	A	109	55.561	58.104	35.858	1.00	15.89
ATOM	839	O	GLU	A	109	55.062	57.376	36.696	1.00	16.10
ATOM	840	CB	GLU	A	109	54.259	59.300	34.091	1.00	18.77
ATOM	841	CG	GLU	A	109	53.234	59.595	35.166	1.00	19.64
ATOM	842	CD	GLU	A	109	52.394	60.875	34.948	1.00	21.63
ATOM	843	OE1	GLU	A	109	52.761	61.761	34.165	1.00	24.76
ATOM	844	OE2	GLU	A	109	51.361	60.960	35.616	1.00	28.24
ATOM	845	N	GLY	A	110	56.507	59.001	36.063	1.00	15.85
ATOM	846	CA	GLY	A	110	57.054	59.240	37.466	1.00	17.20
ATOM	847	C	GLY	A	110	57.499	57.968	38.164	1.00	16.93
ATOM	848	O	GLY	A	110	58.272	57.157	37.598	1.00	16.26
ATOM	849	N	ASP	A	111	57.047	57.749	39.423	1.00	14.38
ATOM	850	CA	ASP	A	111	57.455	56.568	40.177	1.00	14.84
ATOM	851	C	ASP	A	111	56.588	55.369	39.865	1.00	14.72
ATOM	852	O	ASP	A	111	55.888	54.753	40.690	1.00	14.34
ATOM	853	CB	ASP	A	111	57.356	56.953	41.689	1.00	17.05
ATOM	854	CG	ASP	A	111	57.812	55.841	42.614	1.00	19.59
ATOM	855	OD1	ASP	A	111	58.707	55.034	42.277	1.00	20.52
ATOM	856	OD2	ASP	A	111	57.219	55.731	43.714	1.00	19.81
ATOM	857	N	ASN	A	112	56.617	54.987	38.573	1.00	14.68
ATOM	858	CA	ASN	A	112	55.763	53.835	38.157	1.00	16.14
ATOM	859	C	ASN	A	112	54.291	54.049	38.569	1.00	13.02

ATOM	860	O	ASN	A	112	53.609	53.111	39.049	1.00	14.89
ATOM	861	CB	ASN	A	112	56.322	52.431	38.503	1.00	16.17
ATOM	862	CG	ASN	A	112	57.541	52.089	37.656	1.00	18.78
ATOM	863	OD1	ASN	A	112	57.742	52.728	36.605	1.00	17.25
ATOM	864	ND2	ASN	A	112	58.332	51.112	38.079	1.00	15.61
ATOM	865	N	GLU	A	113	53.814	55.286	38.317	1.00	14.05
ATOM	866	CA	GLU	A	113	52.440	55.685	38.605	1.00	15.74
ATOM	867	C	GLU	A	113	51.602	55.432	37.349	1.00	18.95
ATOM	868	O	GLU	A	113	51.844	56.053	36.325	1.00	19.58
ATOM	869	CB	GLU	A	113	52.402	57.167	38.952	1.00	17.38
ATOM	870	CG	GLU	A	113	51.034	57.648	39.454	1.00	20.91
ATOM	871	CD	GLU	A	113	50.594	57.002	40.802	1.00	24.09
ATOM	872	OE1	GLU	A	113	51.358	56.979	41.779	1.00	30.10
ATOM	873	OE2	GLU	A	113	49.450	56.530	40.862	1.00	36.71
ATOM	874	N	MET	A	114	50.624	54.554	37.470	1.00	18.64
ATOM	875	CA	MET	A	114	49.757	54.212	36.305	1.00	20.88
ATOM	876	C	MET	A	114	48.811	55.341	36.028	1.00	27.67
ATOM	877	O	MET	A	114	48.090	55.775	36.930	1.00	27.90
ATOM	878	CB	MET	A	114	48.991	52.925	36.584	1.00	23.89
ATOM	879	CG	MET	A	114	48.173	52.424	35.345	1.00	26.69
ATOM	880	SD	MET	A	114	47.345	50.879	35.650	1.00	29.33
ATOM	881	CE	MET	A	114	48.738	49.883	36.101	1.00	23.75
ATOM	882	N	LYS	A	115	48.790	55.846	34.789	1.00	25.26
ATOM	883	CA	LYS	A	115	47.883	56.943	34.440	1.00	30.27
ATOM	884	C	LYS	A	115	46.430	56.485	34.405	1.00	36.08
ATOM	885	O	LYS	A	115	45.545	57.363	34.605	1.00	41.29
ATOM	886	CB	LYS	A	115	48.251	57.602	33.112	1.00	31.52
ATOM	887	CG	LYS	A	115	49.665	58.100	32.995	1.00	29.39
ATOM	888	CD	LYS	A	115	49.830	58.930	31.710	1.00	35.11
ATOM	889	CE	LYS	A	115	51.281	59.149	31.351	1.00	39.16
ATOM	890	NZ	LYS	A	115	51.445	60.206	30.288	1.00	41.83
ATOM	892	N	MET	B	1	49.295	18.983	11.961	1.00	17.87
ATOM	893	CA	MET	B	1	50.088	19.983	12.674	1.00	15.77
ATOM	894	C	MET	B	1	49.867	21.364	12.128	1.00	18.38
ATOM	895	O	MET	B	1	49.270	21.493	11.014	1.00	16.03
ATOM	896	CB	MET	B	1	51.505	19.597	12.960	1.00	18.15
ATOM	897	CG	MET	B	1	52.312	19.036	11.858	1.00	21.69
ATOM	898	SD	MET	B	1	52.465	20.286	10.552	1.00	24.50
ATOM	899	CE	MET	B	1	53.497	19.234	9.256	1.00	19.90
ATOM	900	N	ILE	B	2	50.273	22.378	12.874	1.00	13.90
ATOM	901	CA	ILE	B	2	50.019	23.771	12.510	1.00	12.73
ATOM	902	C	ILE	B	2	51.265	24.482	12.069	1.00	15.11
ATOM	903	O	ILE	B	2	52.322	24.450	12.698	1.00	13.08
ATOM	904	CB	ILE	B	2	49.400	24.499	13.757	1.00	12.91
ATOM	905	CG1	ILE	B	2	48.119	23.792	14.267	1.00	14.95
ATOM	906	CG2	ILE	B	2	49.218	25.945	13.547	1.00	13.31
ATOM	907	CD1	ILE	B	2	46.943	23.904	13.276	1.00	19.87
ATOM	908	N	ARG	B	3	51.138	25.131	10.910	1.00	11.64
ATOM	909	CA	ARG	B	3	52.229	25.868	10.327	1.00	9.38
ATOM	910	C	ARG	B	3	52.150	27.383	10.524	1.00	8.16
ATOM	911	O	ARG	B	3	51.039	27.931	10.673	1.00	9.82
ATOM	912	CB	ARG	B	3	52.082	25.697	8.760	1.00	11.91
ATOM	913	CG	ARG	B	3	52.248	24.258	8.287	1.00	12.07
ATOM	914	CD	ARG	B	3	53.705	23.876	8.003	1.00	12.41
ATOM	915	NE	ARG	B	3	53.758	22.596	7.334	1.00	12.53
ATOM	916	CZ	ARG	B	3	54.867	21.986	6.901	1.00	11.34
ATOM	917	NH1	ARG	B	3	56.094	22.483	7.125	1.00	11.49
ATOM	918	NH2	ARG	B	3	54.748	20.841	6.167	1.00	11.64
ATOM	919	N	THR	B	4	53.317	28.048	10.501	1.00	11.35
ATOM	920	CA	THR	B	4	53.417	29.519	10.576	1.00	10.99

ATOM	921	C	THR	B	4	53.769	29.941	9.093	1.00	9.80
ATOM	922	O	THR	B	4	54.789	29.551	8.631	1.00	10.46
ATOM	923	CB	THR	B	4	54.502	29.963	11.507	1.00	13.30
ATOM	924	OG1	THR	B	4	54.145	29.451	12.826	1.00	12.86
ATOM	925	CG2	THR	B	4	54.597	31.446	11.593	1.00	11.07
ATOM	926	N	MET	B	5	52.897	30.764	8.525	1.00	10.61
ATOM	927	CA	MET	B	5	53.045	31.215	7.092	1.00	10.17
ATOM	928	C	MET	B	5	53.023	32.709	6.987	1.00	13.79
ATOM	929	O	MET	B	5	52.333	33.412	7.759	1.00	12.14
ATOM	930	CB	MET	B	5	51.799	30.698	6.391	1.00	10.85
ATOM	931	CG	MET	B	5	51.655	29.138	6.389	1.00	13.35
ATOM	932	SD	MET	B	5	52.937	28.173	5.793	1.00	12.31
ATOM	933	CE	MET	B	5	52.760	28.465	3.924	1.00	9.06
ATOM	934	N	LEU	B	6	53.705	33.229	5.939	1.00	11.48
ATOM	935	CA	LEU	B	6	53.676	34.675	5.698	1.00	11.70
ATOM	936	C	LEU	B	6	52.227	35.093	5.344	1.00	15.58
ATOM	937	O	LEU	B	6	51.621	34.549	4.376	1.00	12.84
ATOM	938	CB	LEU	B	6	54.595	34.999	4.516	1.00	11.07
ATOM	939	CG	LEU	B	6	54.561	36.468	4.141	1.00	10.79
ATOM	940	CD1	LEU	B	6	55.327	37.415	5.158	1.00	12.32
ATOM	941	CD2	LEU	B	6	55.228	36.692	2.748	1.00	12.20
ATOM	942	N	GLN	B	7	51.608	36.000	6.115	1.00	11.50
ATOM	943	CA	GLN	B	7	50.275	36.439	5.854	1.00	12.08
ATOM	944	C	GLN	B	7	50.283	37.543	4.772	1.00	13.00
ATOM	945	O	GLN	B	7	49.368	37.573	3.878	1.00	13.76
ATOM	946	CB	GLN	B	7	49.614	37.046	7.144	1.00	13.70
ATOM	947	CG	GLN	B	7	48.181	37.402	7.017	1.00	13.52
ATOM	948	CD	GLN	B	7	47.882	38.740	6.256	1.00	15.62
ATOM	949	OE1	GLN	B	7	46.810	38.816	5.553	1.00	14.96
ATOM	950	NE2	GLN	B	7	48.745	39.780	6.431	1.00	13.51
ATOM	951	N	GLY	B	8	51.235	38.442	4.850	1.00	12.82
ATOM	952	CA	GLY	B	8	51.318	39.567	3.907	1.00	13.57
ATOM	953	C	GLY	B	8	52.519	40.435	4.210	1.00	17.33
ATOM	954	O	GLY	B	8	53.154	40.314	5.278	1.00	16.12
ATOM	955	N	LYS	B	9	52.917	41.301	3.271	1.00	13.73
ATOM	956	CA	LYS	B	9	54.045	42.162	3.517	1.00	14.09
ATOM	957	C	LYS	B	9	53.980	43.423	2.693	1.00	17.41
ATOM	958	O	LYS	B	9	53.290	43.474	1.636	1.00	16.23
ATOM	959	CB	LYS	B	9	55.357	41.484	3.338	1.00	17.25
ATOM	960	CG	LYS	B	9	55.685	41.165	1.849	1.00	16.41
ATOM	961	CD	LYS	B	9	57.128	40.757	1.590	1.00	16.11
ATOM	962	CE	LYS	B	9	57.413	40.363	0.083	1.00	20.64
ATOM	963	NZ	LYS	B	9	58.845	40.122	-0.219	1.00	24.09
ATOM	964	N	LEU	B	10	54.623	44.438	3.206	1.00	14.37
ATOM	965	CA	LEU	B	10	54.793	45.753	2.541	1.00	13.07
ATOM	966	C	LEU	B	10	56.264	45.671	2.117	1.00	17.74
ATOM	967	O	LEU	B	10	57.211	45.651	2.922	1.00	15.88
ATOM	968	CB	LEU	B	10	54.531	46.942	3.473	1.00	12.64
ATOM	969	CG	LEU	B	10	53.125	47.012	4.065	1.00	16.69
ATOM	970	CD1	LEU	B	10	52.972	48.183	5.050	1.00	19.95
ATOM	971	CD2	LEU	B	10	51.998	47.113	2.952	1.00	18.21
ATOM	972	N	HIS	B	11	56.532	45.559	0.795	1.00	15.41
ATOM	973	CA	HIS	B	11	57.852	45.410	0.342	1.00	15.54
ATOM	974	C	HIS	B	11	58.554	46.680	-0.107	1.00	20.36
ATOM	975	O	HIS	B	11	58.088	47.329	-1.109	1.00	19.27
ATOM	976	CB	HIS	B	11	57.855	44.396	-0.897	1.00	17.02
ATOM	977	CG	HIS	B	11	59.222	43.925	-1.277	1.00	20.52
ATOM	978	ND1	HIS	B	11	59.891	42.946	-0.575	1.00	23.10
ATOM	979	CD2	HIS	B	11	60.067	44.321	-2.265	1.00	23.01
ATOM	980	CE1	HIS	B	11	61.084	42.750	-1.109	1.00	22.29

ATOM	981	NE2	HIS	B	11	61.218	43.579	-2.141	1.00	22.03
ATOM	982	N	ARG	B	12	59.636	47.041	0.577	1.00	17.66
ATOM	983	CA	ARG	B	12	60.427	48.202	0.273	1.00	17.87
ATOM	984	C	ARG	B	12	59.755	49.542	0.461	1.00	21.36
ATOM	985	O	ARG	B	12	59.858	50.465	-0.401	1.00	21.72
ATOM	986	CB	ARG	B	12	61.185	48.082	-1.105	1.00	17.27
ATOM	987	CG	ARG	B	12	62.150	46.920	-1.155	1.00	16.85
ATOM	988	CD	ARG	B	12	62.849	46.746	-2.537	1.00	21.64
ATOM	989	NE	ARG	B	12	63.541	47.993	-2.907	1.00	26.91
ATOM	990	CZ	ARG	B	12	64.818	48.252	-2.642	1.00	32.28
ATOM	991	NH1	ARG	B	12	65.345	49.421	-3.011	1.00	32.70
ATOM	992	NH2	ARG	B	12	65.573	47.367	-2.015	1.00	23.04
ATOM	993	N	VAL	B	13	59.082	49.737	1.613	1.00	16.36
ATOM	994	CA	VAL	B	13	58.476	51.010	1.919	1.00	16.81
ATOM	995	C	VAL	B	13	59.568	51.825	2.625	1.00	19.79
ATOM	996	O	VAL	B	13	60.555	51.259	3.103	1.00	21.56
ATOM	997	CB	VAL	B	13	57.262	50.903	2.868	1.00	20.87
ATOM	998	CG1	VAL	B	13	56.117	50.340	2.233	1.00	22.00
ATOM	999	CG2	VAL	B	13	57.614	50.095	4.174	1.00	19.93
ATOM	1000	N	LYS	B	14	59.429	53.148	2.658	1.00	17.58
ATOM	1001	CA	LYS	B	14	60.462	53.955	3.313	1.00	18.29
ATOM	1002	C	LYS	B	14	59.955	54.558	4.631	1.00	17.32
ATOM	1003	O	LYS	B	14	58.811	54.965	4.720	1.00	17.18
ATOM	1004	CB	LYS	B	14	60.958	55.077	2.370	1.00	21.96
ATOM	1005	CG	LYS	B	14	61.928	54.568	1.327	1.00	29.69
ATOM	1006	CD	LYS	B	14	62.379	55.718	0.374	1.00	27.98
ATOM	1007	CE	LYS	B	14	63.251	55.192	-0.769	1.00	33.09
ATOM	1008	NZ	LYS	B	14	62.422	54.676	-1.901	1.00	36.70
ATOM	1009	N	VAL	B	15	60.836	54.550	5.641	1.00	17.61
ATOM	1010	CA	VAL	B	15	60.462	55.122	6.942	1.00	15.98
ATOM	1011	C	VAL	B	15	60.291	56.648	6.751	1.00	18.36
ATOM	1012	O	VAL	B	15	61.155	57.284	6.183	1.00	20.10
ATOM	1013	CB	VAL	B	15	61.537	54.823	7.986	1.00	18.17
ATOM	1014	CG1	VAL	B	15	61.172	55.554	9.332	1.00	19.48
ATOM	1015	CG2	VAL	B	15	61.579	53.284	8.219	1.00	18.97
ATOM	1016	N	THR	B	16	59.195	57.208	7.241	1.00	16.59
ATOM	1017	CA	THR	B	16	58.949	58.657	7.071	1.00	18.46
ATOM	1018	C	THR	B	16	59.061	59.479	8.337	1.00	23.98
ATOM	1019	O	THR	B	16	59.187	60.728	8.286	1.00	23.98
ATOM	1020	CB	THR	B	16	57.537	58.906	6.438	1.00	20.68
ATOM	1021	OG1	THR	B	16	56.495	58.483	7.322	1.00	20.66
ATOM	1022	CG2	THR	B	16	57.407	58.134	5.067	1.00	20.82
ATOM	1023	N	HIS	B	17	59.034	58.811	9.484	1.00	21.79
ATOM	1024	CA	HIS	B	17	59.102	59.539	10.776	1.00	23.09
ATOM	1025	C	HIS	B	17	59.580	58.582	11.852	1.00	25.64
ATOM	1026	O	HIS	B	17	59.398	57.358	11.739	1.00	20.59
ATOM	1027	CB	HIS	B	17	57.630	59.960	11.101	1.00	25.73
ATOM	1028	CG	HIS	B	17	57.436	60.783	12.353	1.00	31.57
ATOM	1029	ND1	HIS	B	17	56.596	60.377	13.379	1.00	34.88
ATOM	1030	CD2	HIS	B	17	57.919	62.000	12.724	1.00	34.96
ATOM	1031	CE1	HIS	B	17	56.589	61.293	14.335	1.00	35.01
ATOM	1032	NE2	HIS	B	17	57.383	62.290	13.966	1.00	35.08
ATOM	1033	N	ALA	B	18	60.189	59.139	12.893	1.00	25.07
ATOM	1034	CA	ALA	B	18	60.673	58.327	14.027	1.00	25.93
ATOM	1035	C	ALA	B	18	60.235	59.122	15.285	1.00	31.11
ATOM	1036	O	ALA	B	18	60.376	60.360	15.314	1.00	33.50
ATOM	1037	CB	ALA	B	18	62.157	58.146	13.972	1.00	27.54
ATOM	1038	N	ASP	B	19	59.643	58.456	16.281	1.00	24.42
ATOM	1039	CA	ASP	B	19	59.162	59.161	17.502	1.00	24.78
ATOM	1040	C	ASP	B	19	59.503	58.342	18.739	1.00	27.05

ATOM	1041	O	ASP	B	19	58.658	57.595	19.257	1.00	24.71
ATOM	1042	CB	ASP	B	19	57.647	59.409	17.384	1.00	25.96
ATOM	1043	CG	ASP	B	19	57.052	60.183	18.572	1.00	34.10
ATOM	1044	OD1	ASP	B	19	57.807	60.624	19.466	1.00	34.04
ATOM	1045	OD2	ASP	B	19	55.800	60.351	18.593	1.00	38.22
ATOM	1046	N	LEU	B	20	60.742	58.494	19.199	1.00	25.80
ATOM	1047	CA	LEU	B	20	61.238	57.779	20.364	1.00	24.85
ATOM	1048	C	LEU	B	20	60.390	57.962	21.616	1.00	27.59
ATOM	1049	O	LEU	B	20	60.129	56.981	22.335	1.00	26.06
ATOM	1050	CB	LEU	B	20	62.689	58.208	20.666	1.00	25.72
ATOM	1051	CG	LEU	B	20	63.459	57.525	21.809	1.00	29.24
ATOM	1052	CD1	LEU	B	20	63.844	56.100	21.431	1.00	28.84
ATOM	1053	CD2	LEU	B	20	64.720	58.345	22.159	1.00	29.15
ATOM	1054	N	HIS	B	21	59.981	59.207	21.878	1.00	28.61
ATOM	1055	CA	HIS	B	21	59.155	59.572	23.074	1.00	30.90
ATOM	1056	C	HIS	B	21	57.680	59.351	23.007	1.00	36.12
ATOM	1057	O	HIS	B	21	56.915	59.806	23.896	1.00	35.00
ATOM	1058	CB	HIS	B	21	59.509	60.991	23.549	1.00	32.76
ATOM	1059	CG	HIS	B	21	60.950	61.157	23.845	1.00	36.81
ATOM	1060	ND1	HIS	B	21	61.792	61.941	23.086	1.00	39.48
ATOM	1061	CD2	HIS	B	21	61.731	60.556	24.776	1.00	38.76
ATOM	1062	CE1	HIS	B	21	63.025	61.847	23.564	1.00	38.26
ATOM	1063	NE2	HIS	B	21	63.014	61.014	24.588	1.00	38.36
ATOM	1064	N	TYR	B	22	57.270	58.641	21.975	1.00	33.13
ATOM	1065	CA	TYR	B	22	55.874	58.333	21.767	1.00	33.14
ATOM	1066	C	TYR	B	22	55.136	57.743	22.985	1.00	37.60
ATOM	1067	O	TYR	B	22	55.697	56.936	23.774	1.00	32.76
ATOM	1068	CB	TYR	B	22	55.794	57.254	20.681	1.00	33.35
ATOM	1069	CG	TYR	B	22	54.410	57.005	20.169	1.00	35.03
ATOM	1070	CD1	TYR	B	22	53.728	58.003	19.481	1.00	36.82
ATOM	1071	CD2	TYR	B	22	53.772	55.794	20.385	1.00	35.58
ATOM	1072	CE1	TYR	B	22	52.442	57.795	19.013	1.00	37.35
ATOM	1073	CE2	TYR	B	22	52.491	55.577	19.914	1.00	36.01
ATOM	1074	CZ	TYR	B	22	51.834	56.569	19.229	1.00	42.70
ATOM	1075	OH	TYR	B	22	50.542	56.288	18.772	1.00	46.65
ATOM	1076	N	GLU	B	23	53.877	58.126	23.092	1.00	39.24
ATOM	1077	CA	GLU	B	23	52.991	57.636	24.122	1.00	42.44
ATOM	1078	C	GLU	B	23	51.673	57.203	23.428	1.00	47.01
ATOM	1079	O	GLU	B	23	50.884	58.032	23.017	1.00	48.53
ATOM	1080	CB	GLU	B	23	52.723	58.677	25.211	1.00	44.81
ATOM	1081	CG	GLU	B	23	51.620	58.234	26.155	1.00	53.00
ATOM	1082	CD	GLU	B	23	51.690	58.900	27.515	1.00	63.57
ATOM	1083	OE1	GLU	B	23	52.173	60.058	27.596	1.00	70.57
ATOM	1084	OE2	GLU	B	23	51.237	58.268	28.501	1.00	49.95
ATOM	1085	N	GLY	B	24	51.453	55.900	23.305	1.00	43.35
ATOM	1086	CA	GLY	B	24	50.234	55.411	22.678	1.00	47.63
ATOM	1087	C	GLY	B	24	50.321	53.939	22.257	1.00	49.81
ATOM	1088	O	GLY	B	24	50.860	53.127	23.028	1.00	43.71
ATOM	1089	OH	GLY	B	24	49.852	53.595	21.143	1.00	78.26
ATOM	1090	C	PVL	B	25	55.590	51.160	16.243	1.00	18.29
ATOM	1091	O	PVL	B	25	56.587	51.766	16.023	1.00	21.21
ATOM	1092	CA	PVL	B	25	55.340	50.687	17.625	1.00	27.46
ATOM	1093	CB	PVL	B	25	54.143	49.829	17.834	1.00	25.35
ATOM	1094	ON	PVL	B	25	56.135	50.957	18.541	1.00	33.71
ATOM	1095	N	CYS	B	26	54.735	50.714	15.217	1.00	15.60
ATOM	1096	CA	CYS	B	26	54.985	51.203	13.855	1.00	16.64
ATOM	1097	CB	CYS	B	26	55.756	50.146	13.029	1.00	14.30
ATOM	1098	SG	CYS	B	26	56.010	50.798	11.325	1.00	18.05
ATOM	1099	C	CYS	B	26	53.636	51.600	13.281	1.00	14.55
ATOM	1100	O	CYS	B	26	52.716	50.778	13.121	1.00	16.28

ATOM	1101	N	ALA	B	27	53.472	52.925	13.012	1.00	15.46
ATOM	1102	CA	ALA	B	27	52.197	53.479	12.457	1.00	15.63
ATOM	1103	C	ALA	B	27	52.328	53.470	10.917	1.00	15.10
ATOM	1104	O	ALA	B	27	53.303	53.924	10.380	1.00	15.77
ATOM	1105	CB	ALA	B	27	51.919	54.908	12.948	1.00	16.71
ATOM	1106	N	ILE	B	28	51.301	52.924	10.300	1.00	14.23
ATOM	1107	CA	ILE	B	28	51.286	52.712	8.846	1.00	14.71
ATOM	1108	C	ILE	B	28	49.989	53.151	8.224	1.00	17.41
ATOM	1109	O	ILE	B	28	48.913	52.880	8.714	1.00	16.90
ATOM	1110	CB	ILE	B	28	51.404	51.141	8.665	1.00	16.58
ATOM	1111	CG1	ILE	B	28	52.699	50.640	9.314	1.00	16.36
ATOM	1112	CG2	ILE	B	28	51.329	50.765	7.154	1.00	15.52
ATOM	1113	CD1	ILE	B	28	52.708	49.114	9.667	1.00	18.68
ATOM	1114	N	ASP	B	29	50.128	53.872	7.090	1.00	16.97
ATOM	1115	CA	ASP	B	29	48.943	54.364	6.337	1.00	18.01
ATOM	1116	C	ASP	B	29	47.927	53.186	6.186	1.00	17.51
ATOM	1117	O	ASP	B	29	48.339	52.095	5.725	1.00	15.93
ATOM	1118	CB	ASP	B	29	49.481	54.766	4.949	1.00	18.64
ATOM	1119	CG	ASP	B	29	48.383	55.304	3.960	1.00	21.55
ATOM	1120	OD1	ASP	B	29	47.171	55.003	4.082	1.00	21.30
ATOM	1121	OD2	ASP	B	29	48.831	56.051	3.034	1.00	22.85
ATOM	1122	N	GLN	B	30	46.665	53.404	6.579	1.00	17.64
ATOM	1123	CA	GLN	B	30	45.593	52.389	6.498	1.00	16.64
ATOM	1124	C	GLN	B	30	45.497	51.773	5.101	1.00	20.42
ATOM	1125	O	GLN	B	30	45.212	50.578	4.991	1.00	19.64
ATOM	1126	CB	GLN	B	30	44.231	52.918	6.947	1.00	19.10
ATOM	1127	CG	GLN	B	30	43.138	51.881	6.990	1.00	20.18
ATOM	1128	CD	GLN	B	30	43.422	50.807	8.020	1.00	24.27
ATOM	1129	OE1	GLN	B	30	43.624	51.129	9.221	1.00	20.83
ATOM	1130	NE2	GLN	B	30	43.418	49.525	7.584	1.00	20.72
ATOM	1131	N	ASP	B	31	45.765	52.541	4.034	1.00	19.98
ATOM	1132	CA	ASP	B	31	45.692	51.922	2.700	1.00	20.52
ATOM	1133	C	ASP	B	31	46.711	50.794	2.519	1.00	19.87
ATOM	1134	O	ASP	B	31	46.458	49.781	1.783	1.00	20.49
ATOM	1135	CB	ASP	B	31	45.971	52.970	1.621	1.00	20.56
ATOM	1136	CG	ASP	B	31	44.751	53.787	1.281	1.00	27.59
ATOM	1137	OD1	ASP	B	31	43.596	53.382	1.538	1.00	27.63
ATOM	1138	OD2	ASP	B	31	44.990	54.926	0.798	1.00	25.47
ATOM	1139	N	PHE	B	32	47.886	50.935	3.170	1.00	17.26
ATOM	1140	CA	PHE	B	32	48.951	49.962	3.088	1.00	16.13
ATOM	1141	C	PHE	B	32	48.525	48.723	3.890	1.00	15.84
ATOM	1142	O	PHE	B	32	48.690	47.554	3.430	1.00	15.43
ATOM	1143	CB	PHE	B	32	50.278	50.479	3.670	1.00	17.62
ATOM	1144	CG	PHE	B	32	50.847	51.723	2.976	1.00	18.64
ATOM	1145	CD1	PHE	B	32	50.236	52.299	1.842	1.00	20.38
ATOM	1146	CD2	PHE	B	32	52.019	52.292	3.473	1.00	21.28
ATOM	1147	CE1	PHE	B	32	50.828	53.473	1.249	1.00	21.62
ATOM	1148	CE2	PHE	B	32	52.587	53.413	2.908	1.00	24.06
ATOM	1149	CZ	PHE	B	32	51.988	54.006	1.779	1.00	22.14
ATOM	1150	N	LEU	B	33	47.989	48.981	5.086	1.00	15.62
ATOM	1151	CA	LEU	B	33	47.526	47.856	5.919	1.00	15.62
ATOM	1152	C	LEU	B	33	46.481	47.031	5.124	1.00	14.56
ATOM	1153	O	LEU	B	33	46.534	45.810	5.106	1.00	15.50
ATOM	1154	CB	LEU	B	33	46.899	48.361	7.221	1.00	15.46
ATOM	1155	CG	LEU	B	33	47.899	49.072	8.189	1.00	17.68
ATOM	1156	CD1	LEU	B	33	47.114	49.554	9.450	1.00	18.11
ATOM	1157	CD2	LEU	B	33	48.993	48.086	8.627	1.00	17.59
ATOM	1158	N	ASP	B	34	45.530	47.724	4.466	1.00	15.47
ATOM	1159	CA	ASP	B	34	44.461	47.090	3.695	1.00	15.42
ATOM	1160	C	ASP	B	34	45.018	46.177	2.609	1.00	15.50

ATOM	1161	O	ASP	B	34	44.542	45.082	2.444	1.00	16.94
ATOM	1162	CB	ASP	B	34	43.604	48.177	3.031	1.00	16.78
ATOM	1163	CG	ASP	B	34	42.649	48.846	3.990	1.00	21.53
ATOM	1164	OD1	ASP	B	34	42.574	48.461	5.192	1.00	22.41
ATOM	1165	OD2	ASP	B	34	41.944	49.809	3.549	1.00	24.39
ATOM	1166	N	ALA	B	35	46.013	46.650	1.875	1.00	15.30
ATOM	1167	CA	ALA	B	35	46.623	45.864	0.804	1.00	16.57
ATOM	1168	C	ALA	B	35	47.378	44.636	1.289	1.00	18.73
ATOM	1169	O	ALA	B	35	47.387	43.587	0.644	1.00	19.02
ATOM	1170	CB	ALA	B	35	47.576	46.726	-0.042	1.00	18.18
ATOM	1171	N	ALA	B	36	48.063	44.784	2.448	1.00	15.77
ATOM	1172	CA	ALA	B	36	48.818	43.688	2.949	1.00	14.01
ATOM	1173	C	ALA	B	36	48.015	42.756	3.920	1.00	12.66
ATOM	1174	O	ALA	B	36	48.612	41.710	4.327	1.00	15.97
ATOM	1175	CB	ALA	B	36	50.083	44.221	3.681	1.00	15.98
ATOM	1176	N	GLY	B	37	46.798	43.130	4.266	1.00	12.31
ATOM	1177	CA	GLY	B	37	45.973	42.352	5.150	1.00	12.99
ATOM	1178	C	GLY	B	37	46.496	42.432	6.606	1.00	13.99
ATOM	1179	O	GLY	B	37	46.069	41.557	7.415	1.00	13.49
ATOM	1180	N	ILE	B	38	47.307	43.444	6.904	1.00	13.30
ATOM	1181	CA	ILE	B	38	47.864	43.618	8.310	1.00	11.90
ATOM	1182	C	ILE	B	38	46.839	44.382	9.121	1.00	13.73
ATOM	1183	O	ILE	B	38	46.308	45.399	8.700	1.00	13.87
ATOM	1184	CB	ILE	B	38	49.184	44.279	8.258	1.00	12.06
ATOM	1185	CG1	ILE	B	38	50.228	43.360	7.542	1.00	13.02
ATOM	1186	CG2	ILE	B	38	49.697	44.582	9.755	1.00	11.46
ATOM	1187	CD1	ILE	B	38	51.570	43.996	7.284	1.00	14.92
ATOM	1188	N	LEU	B	39	46.564	43.916	10.371	1.00	11.75
ATOM	1189	CA	LEU	B	39	45.578	44.546	11.229	1.00	11.57
ATOM	1190	C	LEU	B	39	46.194	45.436	12.297	1.00	13.60
ATOM	1191	O	LEU	B	39	47.314	45.212	12.681	1.00	12.83
ATOM	1192	CB	LEU	B	39	44.793	43.478	11.979	1.00	11.62
ATOM	1193	CG	LEU	B	39	44.184	42.300	11.176	1.00	13.66
ATOM	1194	CD1	LEU	B	39	43.446	41.373	12.104	1.00	15.79
ATOM	1195	CD2	LEU	B	39	43.241	42.956	10.120	1.00	15.29
ATOM	1196	N	GLU	B	40	45.452	46.455	12.667	1.00	14.52
ATOM	1197	CA	GLU	B	40	45.908	47.316	13.786	1.00	14.56
ATOM	1198	C	GLU	B	40	46.034	46.318	14.996	1.00	14.90
ATOM	1199	O	GLU	B	40	45.194	45.428	15.204	1.00	13.14
ATOM	1200	CB	GLU	B	40	44.819	48.341	14.096	1.00	17.43
ATOM	1201	CG	GLU	B	40	45.175	49.769	13.693	1.00	36.71
ATOM	1202	CD	GLU	B	40	44.728	50.776	14.770	1.00	43.99
ATOM	1203	OE1	GLU	B	40	43.514	50.732	15.112	1.00	33.64
ATOM	1204	OE2	GLU	B	40	45.573	51.603	15.285	1.00	23.74
ATOM	1205	N	ASN	B	41	47.136	46.514	15.758	1.00	12.38
ATOM	1206	CA	ASN	B	41	47.457	45.691	16.951	1.00	12.93
ATOM	1207	C	ASN	B	41	48.019	44.334	16.656	1.00	15.81
ATOM	1208	O	ASN	B	41	48.283	43.527	17.534	1.00	13.21
ATOM	1209	CB	ASN	B	41	46.298	45.648	17.922	1.00	14.28
ATOM	1210	CG	ASN	B	41	45.966	47.041	18.493	1.00	12.10
ATOM	1211	OD1	ASN	B	41	46.860	47.804	18.856	1.00	16.64
ATOM	1212	ND2	ASN	B	41	44.680	47.382	18.491	1.00	15.27
ATOM	1213	N	GLU	B	42	48.244	44.017	15.384	1.00	10.98
ATOM	1214	CA	GLU	B	42	48.831	42.744	15.033	1.00	9.74
ATOM	1215	C	GLU	B	42	50.356	42.767	15.148	1.00	9.74
ATOM	1216	O	GLU	B	42	51.026	43.784	14.869	1.00	10.17
ATOM	1217	CB	GLU	B	42	48.499	42.388	13.482	1.00	10.40
ATOM	1218	CG	GLU	B	42	48.990	40.990	13.056	1.00	10.03
ATOM	1219	CD	GLU	B	42	48.652	40.661	11.573	1.00	13.25
ATOM	1220	OE1	GLU	B	42	48.260	41.628	10.893	1.00	15.16

ATOM	1221	OE2	GLU	B	42	48.788	39.493	11.198	1.00	12.03
ATOM	1222	N	ALA	B	43	50.947	41.634	15.574	1.00	9.51
ATOM	1223	CA	ALA	B	43	52.384	41.493	15.647	1.00	10.88
ATOM	1224	C	ALA	B	43	52.996	41.666	14.214	1.00	10.85
ATOM	1225	O	ALA	B	43	52.435	41.054	13.263	1.00	11.54
ATOM	1226	CB	ALA	B	43	52.772	40.069	16.175	1.00	12.49
ATOM	1227	N	ILE	B	44	54.041	42.408	14.075	1.00	11.86
ATOM	1228	CA	ILE	B	44	54.719	42.557	12.737	1.00	11.02
ATOM	1229	C	ILE	B	44	56.251	42.437	12.901	1.00	13.51
ATOM	1230	O	ILE	B	44	56.824	42.780	13.996	1.00	13.63
ATOM	1231	CB	ILE	B	44	54.386	43.905	12.029	1.00	12.21
ATOM	1232	CG1	ILE	B	44	54.727	45.106	12.987	1.00	12.04
ATOM	1233	CG2	ILE	B	44	52.925	43.894	11.585	1.00	14.58
ATOM	1234	CD1	ILE	B	44	54.477	46.487	12.346	1.00	12.27
ATOM	1235	N	ASP	B	45	56.970	41.986	11.865	1.00	10.42
ATOM	1236	CA	ASP	B	45	58.401	41.882	11.844	1.00	10.06
ATOM	1237	C	ASP	B	45	58.826	42.973	10.843	1.00	14.23
ATOM	1238	O	ASP	B	45	58.174	43.130	9.772	1.00	14.99
ATOM	1239	CB	ASP	B	45	58.893	40.494	11.379	1.00	12.39
ATOM	1240	CG	ASP	B	45	58.410	39.394	12.277	1.00	15.51
ATOM	1241	OD1	ASP	B	45	58.325	39.655	13.536	1.00	15.80
ATOM	1242	OD2	ASP	B	45	58.044	38.297	11.812	1.00	15.67
ATOM	1243	N	ILE	B	46	59.874	43.711	11.152	1.00	10.63
ATOM	1244	CA	ILE	B	46	60.402	44.798	10.315	1.00	10.58
ATOM	1245	C	ILE	B	46	61.845	44.462	10.039	1.00	14.80
ATOM	1246	O	ILE	B	46	62.670	44.242	10.926	1.00	13.14
ATOM	1247	CB	ILE	B	46	60.237	46.173	10.981	1.00	12.68
ATOM	1248	CG1	ILE	B	46	58.759	46.398	11.267	1.00	11.97
ATOM	1249	CG2	ILE	B	46	60.843	47.266	10.035	1.00	14.01
ATOM	1250	CD1	ILE	B	46	58.431	47.842	11.715	1.00	17.51
ATOM	1251	N	TRP	B	47	62.185	44.361	8.719	1.00	11.09
ATOM	1252	CA	TRP	B	47	63.488	43.982	8.256	1.00	12.91
ATOM	1253	C	TRP	B	47	64.025	45.208	7.488	1.00	18.14
ATOM	1254	O	TRP	B	47	63.436	45.628	6.467	1.00	16.83
ATOM	1255	CB	TRP	B	47	63.352	42.731	7.340	1.00	12.75
ATOM	1256	CG	TRP	B	47	62.711	41.546	8.024	1.00	12.68
ATOM	1257	CD1	TRP	B	47	62.891	41.157	9.370	1.00	13.80
ATOM	1258	CD2	TRP	B	47	61.810	40.606	7.470	1.00	12.97
ATOM	1259	NE1	TRP	B	47	62.133	40.068	9.635	1.00	12.97
ATOM	1260	CE2	TRP	B	47	61.449	39.686	8.500	1.00	14.42
ATOM	1261	CE3	TRP	B	47	61.195	40.476	6.207	1.00	14.96
ATOM	1262	CZ2	TRP	B	47	60.573	38.635	8.298	1.00	14.53
ATOM	1263	CZ3	TRP	B	47	60.351	39.440	5.994	1.00	16.02
ATOM	1264	CH2	TRP	B	47	60.033	38.509	7.012	1.00	16.49
ATOM	1265	N	ASN	B	48	65.081	45.816	8.024	1.00	15.37
ATOM	1266	CA	ASN	B	48	65.648	47.056	7.466	1.00	15.56
ATOM	1267	C	ASN	B	48	66.662	46.765	6.393	1.00	16.84
ATOM	1268	O	ASN	B	48	67.746	46.284	6.662	1.00	15.08
ATOM	1269	CB	ASN	B	48	66.293	47.841	8.654	1.00	14.22
ATOM	1270	CG	ASN	B	48	66.594	49.267	8.309	1.00	19.83
ATOM	1271	OD1	ASN	B	48	67.100	49.532	7.211	1.00	17.68
ATOM	1272	ND2	ASN	B	48	66.291	50.207	9.205	1.00	18.60
ATOM	1273	N	VAL	B	49	66.292	47.051	5.125	1.00	16.35
ATOM	1274	CA	VAL	B	49	67.188	46.806	4.002	1.00	16.91
ATOM	1275	C	VAL	B	49	68.418	47.753	4.002	1.00	18.54
ATOM	1276	O	VAL	B	49	69.539	47.390	3.566	1.00	19.45
ATOM	1277	CB	VAL	B	49	66.442	47.003	2.694	1.00	20.06
ATOM	1278	CG1	VAL	B	49	67.380	46.691	1.524	1.00	21.67
ATOM	1279	CG2	VAL	B	49	65.196	46.106	2.650	1.00	18.68
ATOM	1280	N	THR	B	50	68.196	48.964	4.504	1.00	17.72

ATOM	1281	CA	THR	B	50	69.290	49.926	4.552	1.00	18.92
ATOM	1282	C	THR	B	50	70.403	49.565	5.528	1.00	20.97
ATOM	1283	O	THR	B	50	71.593	49.537	5.172	1.00	20.06
ATOM	1284	CB	THR	B	50	68.764	51.325	4.851	1.00	19.40
ATOM	1285	OG1	THR	B	50	67.798	51.708	3.856	1.00	19.82
ATOM	1286	CG2	THR	B	50	69.931	52.390	4.950	1.00	21.30
ATOM	1287	N	ASN	B	51	70.022	49.279	6.788	1.00	17.46
ATOM	1288	CA	ASN	B	51	71.032	48.962	7.814	1.00	18.39
ATOM	1289	C	ASN	B	51	71.132	47.525	8.327	1.00	19.48
ATOM	1290	O	ASN	B	51	71.970	47.226	9.183	1.00	19.00
ATOM	1291	CB	ASN	B	51	70.913	49.949	8.998	1.00	18.51
ATOM	1292	CG	ASN	B	51	69.679	49.690	9.874	1.00	22.35
ATOM	1293	OD1	ASN	B	51	69.028	48.659	9.772	1.00	17.21
ATOM	1294	ND2	ASN	B	51	69.349	50.649	10.715	1.00	21.24
ATOM	1295	N	GLY	B	52	70.282	46.636	7.807	1.00	15.50
ATOM	1296	CA	GLY	B	52	70.231	45.232	8.164	1.00	14.95
ATOM	1297	C	GLY	B	52	69.601	44.846	9.523	1.00	14.04
ATOM	1298	O	GLY	B	52	69.541	43.629	9.815	1.00	16.62
ATOM	1299	N	LYS	B	53	69.153	45.837	10.279	1.00	14.08
ATOM	1300	CA	LYS	B	53	68.540	45.457	11.593	1.00	14.38
ATOM	1301	C	LYS	B	53	67.239	44.729	11.349	1.00	15.94
ATOM	1302	O	LYS	B	53	66.565	44.973	10.344	1.00	16.45
ATOM	1303	CB	LYS	B	53	68.311	46.698	12.463	1.00	14.22
ATOM	1304	CG	LYS	B	53	69.654	47.303	12.877	1.00	16.49
ATOM	1305	CD	LYS	B	53	69.457	48.540	13.748	1.00	19.28
ATOM	1306	CE	LYS	B	53	70.801	49.177	14.108	1.00	26.70
ATOM	1307	NZ	LYS	B	53	70.585	50.475	14.799	1.00	29.14
ATOM	1308	N	ARG	B	54	66.839	43.849	12.303	1.00	12.88
ATOM	1309	CA	ARG	B	54	65.612	43.091	12.229	1.00	11.93
ATOM	1310	C	ARG	B	54	64.954	43.162	13.592	1.00	14.91
ATOM	1311	O	ARG	B	54	65.646	42.907	14.590	1.00	15.98
ATOM	1312	CB	ARG	B	54	65.862	41.628	11.855	1.00	13.59
ATOM	1313	CG	ARG	B	54	66.751	41.516	10.564	1.00	14.24
ATOM	1314	CD	ARG	B	54	67.058	40.054	10.159	1.00	13.75
ATOM	1315	NE	ARG	B	54	65.931	39.313	9.621	1.00	13.94
ATOM	1316	CZ	ARG	B	54	65.562	39.372	8.330	1.00	16.69
ATOM	1317	NH1	ARG	B	54	66.281	40.180	7.510	1.00	13.80
ATOM	1318	NH2	ARG	B	54	64.520	38.644	7.857	1.00	13.52
ATOM	1319	N	PHE	B	55	63.707	43.548	13.634	1.00	12.40
ATOM	1320	CA	PHE	B	55	63.013	43.648	14.924	1.00	13.30
ATOM	1321	C	PHE	B	55	61.564	43.314	14.815	1.00	18.51
ATOM	1322	O	PHE	B	55	61.017	43.231	13.703	1.00	16.08
ATOM	1323	CB	PHE	B	55	63.302	44.986	15.586	1.00	13.02
ATOM	1324	CG	PHE	B	55	62.735	46.165	14.864	1.00	14.95
ATOM	1325	CD1	PHE	B	55	63.436	46.742	13.782	1.00	15.75
ATOM	1326	CD2	PHE	B	55	61.514	46.740	15.273	1.00	15.13
ATOM	1327	CE1	PHE	B	55	62.892	47.912	13.106	1.00	17.56
ATOM	1328	CE2	PHE	B	55	60.996	47.844	14.615	1.00	17.23
ATOM	1329	CZ	PHE	B	55	61.713	48.427	13.528	1.00	16.09
ATOM	1330	N	SER	B	56	60.880	43.095	15.940	1.00	12.78
ATOM	1331	CA	SER	B	56	59.482	42.752	15.962	1.00	12.18
ATOM	1332	C	SER	B	56	58.741	43.706	16.846	1.00	15.48
ATOM	1333	O	SER	B	56	59.258	44.045	17.916	1.00	14.26
ATOM	1334	CB	SER	B	56	59.222	41.336	16.394	1.00	13.68
ATOM	1335	OG	SER	B	56	59.880	40.377	15.532	1.00	18.10
ATOM	1336	N	THR	B	57	57.570	44.140	16.428	1.00	11.29
ATOM	1337	CA	THR	B	57	56.749	45.129	17.169	1.00	11.02
ATOM	1338	C	THR	B	57	55.256	44.860	16.831	1.00	11.10
ATOM	1339	O	THR	B	57	54.854	43.697	16.649	1.00	10.41
ATOM	1340	CB	THR	B	57	57.270	46.560	16.849	1.00	13.63

ATOM	1341	OG1	THR	B	57	56.492	47.529	17.575	1.00	16.82
ATOM	1342	CG2	THR	B	57	57.073	46.896	15.328	1.00	16.40
ATOM	1343	N	TYR	B	58	54.424	45.890	16.747	1.00	11.85
ATOM	1344	CA	TYR	B	58	52.995	45.709	16.405	1.00	11.66
ATOM	1345	C	TYR	B	58	52.572	46.896	15.567	1.00	14.10
ATOM	1346	O	TYR	B	58	53.194	47.962	15.639	1.00	12.80
ATOM	1347	CB	TYR	B	58	52.072	45.475	17.632	1.00	13.66
ATOM	1348	CG	TYR	B	58	51.879	46.659	18.537	1.00	14.03
ATOM	1349	CD1	TYR	B	58	52.768	46.908	19.611	1.00	14.60
ATOM	1350	CD2	TYR	B	58	50.836	47.529	18.362	1.00	14.69
ATOM	1351	CE1	TYR	B	58	52.596	48.015	20.420	1.00	14.59
ATOM	1352	CE2	TYR	B	58	50.645	48.649	19.199	1.00	16.85
ATOM	1353	CZ	TYR	B	58	51.546	48.875	20.222	1.00	21.58
ATOM	1354	OH	TYR	B	58	51.493	49.934	21.108	1.00	22.59
ATOM	1355	N	ALA	B	59	51.536	46.705	14.748	1.00	12.25
ATOM	1356	CA	ALA	B	59	51.078	47.769	13.891	1.00	12.10
ATOM	1357	C	ALA	B	59	50.067	48.702	14.494	1.00	14.08
ATOM	1358	O	ALA	B	59	49.190	48.297	15.241	1.00	13.85
ATOM	1359	CB	ALA	B	59	50.435	47.110	12.626	1.00	13.24
ATOM	1360	N	ILE	B	60	50.148	49.990	14.096	1.00	15.08
ATOM	1361	CA	ILE	B	60	49.231	51.025	14.514	1.00	17.01
ATOM	1362	C	ILE	B	60	48.729	51.687	13.195	1.00	16.03
ATOM	1363	O	ILE	B	60	49.522	51.850	12.286	1.00	16.17
ATOM	1364	CB	ILE	B	60	50.004	52.105	15.349	1.00	20.97
ATOM	1365	CG1	ILE	B	60	50.363	51.533	16.724	1.00	23.49
ATOM	1366	CG2	ILE	B	60	49.155	53.362	15.569	1.00	23.18
ATOM	1367	CD1	ILE	B	60	51.454	52.337	17.451	1.00	26.91
ATOM	1368	N	ALA	B	61	47.449	52.016	13.107	1.00	16.21
ATOM	1369	CA	ALA	B	61	46.948	52.655	11.878	1.00	17.99
ATOM	1370	C	ALA	B	61	47.328	54.129	11.847	1.00	20.83
ATOM	1371	O	ALA	B	61	47.221	54.819	12.875	1.00	20.99
ATOM	1372	CB	ALA	B	61	45.481	52.541	11.804	1.00	19.35
ATOM	1373	N	ALA	B	62	47.721	54.613	10.665	1.00	17.91
ATOM	1374	CA	ALA	B	62	48.040	56.043	10.407	1.00	17.67
ATOM	1375	C	ALA	B	62	46.962	56.453	9.380	1.00	23.91
ATOM	1376	O	ALA	B	62	46.335	55.614	8.745	1.00	22.36
ATOM	1377	CB	ALA	B	62	49.400	56.238	9.833	1.00	18.45
ATOM	1378	N	GLU	B	63	46.756	57.756	9.246	1.00	22.90
ATOM	1379	CA	GLU	B	63	45.759	58.312	8.358	1.00	23.71
ATOM	1380	C	GLU	B	63	45.824	57.781	6.943	1.00	23.19
ATOM	1381	O	GLU	B	63	46.894	57.737	6.345	1.00	22.01
ATOM	1382	CB	GLU	B	63	45.919	59.835	8.343	1.00	25.20
ATOM	1383	CG	GLU	B	63	44.902	60.517	7.444	1.00	31.69
ATOM	1384	CD	GLU	B	63	44.852	61.991	7.708	1.00	54.65
ATOM	1385	OE1	GLU	B	63	44.033	62.414	8.559	1.00	50.68
ATOM	1386	OE2	GLU	B	63	45.642	62.719	7.072	1.00	49.85
ATOM	1387	N	ARG	B	64	44.657	57.412	6.411	1.00	23.54
ATOM	1388	CA	ARG	B	64	44.564	56.896	5.065	1.00	24.49
ATOM	1389	C	ARG	B	64	45.068	57.940	4.059	1.00	29.91
ATOM	1390	O	ARG	B	64	44.635	59.103	4.101	1.00	30.10
ATOM	1391	CB	ARG	B	64	43.116	56.548	4.739	1.00	24.54
ATOM	1392	CG	ARG	B	64	42.977	55.708	3.502	1.00	33.44
ATOM	1393	CD	ARG	B	64	41.521	55.461	3.169	1.00	30.76
ATOM	1394	NE	ARG	B	64	40.824	54.612	4.127	1.00	27.92
ATOM	1395	CZ	ARG	B	64	41.003	53.288	4.241	1.00	30.52
ATOM	1396	NH1	ARG	B	64	41.878	52.653	3.470	1.00	26.37
ATOM	1397	NH2	ARG	B	64	40.302	52.609	5.131	1.00	30.42
ATOM	1398	N	GLY	B	65	45.967	57.544	3.177	1.00	27.07
ATOM	1399	CA	GLY	B	65	46.485	58.475	2.170	1.00	26.85
ATOM	1400	C	GLY	B	65	47.687	59.292	2.603	1.00	30.69

ATOM	1401	O	GLY	B	65	48.287	59.983	1.789	1.00	31.19
ATOM	1402	N	SER	B	66	48.069	59.183	3.874	1.00	25.88
ATOM	1403	CA	SER	B	66	49.215	59.916	4.387	1.00	24.31
ATOM	1404	C	SER	B	66	50.565	59.353	3.903	1.00	28.10
ATOM	1405	O	SER	B	66	51.589	60.044	3.898	1.00	29.06
ATOM	1406	CB	SER	B	66	49.182	59.888	5.929	1.00	25.33
ATOM	1407	OG	SER	B	66	49.450	58.548	6.422	1.00	25.27
ATOM	1408	N	ARG	B	67	50.576	58.055	3.539	1.00	21.92
ATOM	1409	CA	ARG	B	67	51.780	57.368	3.106	1.00	20.64
ATOM	1410	C	ARG	B	67	52.867	57.306	4.205	1.00	21.33
ATOM	1411	O	ARG	B	67	54.033	57.113	3.932	1.00	23.88
ATOM	1412	CB	ARG	B	67	52.272	57.896	-1.753	1.00	24.90
ATOM	1413	CG	ARG	B	67	51.094	57.832	0.749	1.00	34.18
ATOM	1414	CD	ARG	B	67	51.498	57.942	-0.692	1.00	41.97
ATOM	1415	NE	ARG	B	67	51.642	59.344	-1.083	1.00	42.73
ATOM	1416	CZ	ARG	B	67	50.665	60.252	-1.300	1.00	50.11
ATOM	1417	NH1	ARG	B	67	49.347	60.005	-1.191	1.00	32.87
ATOM	1418	NH2	ARG	B	67	51.053	61.472	-1.652	1.00	35.89
ATOM	1419	N	ILE	B	68	52.404	57.413	5.449	1.00	20.99
ATOM	1420	CA	ILE	B	68	53.313	57.374	6.590	1.00	19.82
ATOM	1421	C	ILE	B	68	53.722	55.943	7.025	1.00	18.74
ATOM	1422	O	ILE	B	68	52.928	54.964	6.944	1.00	18.59
ATOM	1423	CB	ILE	B	68	52.613	58.021	7.843	1.00	22.72
ATOM	1424	CG1	ILE	B	68	52.569	59.567	7.775	1.00	22.79
ATOM	1425	CG2	ILE	B	68	53.272	57.570	9.182	1.00	23.66
ATOM	1426	CD1	ILE	B	68	51.511	60.133	8.696	1.00	24.22
ATOM	1427	N	ILE	B	69	54.953	55.877	7.455	1.00	17.03
ATOM	1428	CA	ILE	B	69	55.592	54.662	8.057	1.00	16.07
ATOM	1429	C	ILE	B	69	56.398	55.328	9.218	1.00	18.47
ATOM	1430	O	ILE	B	69	57.495	55.875	9.001	1.00	19.41
ATOM	1431	CB	ILE	B	69	56.579	53.927	7.167	1.00	17.97
ATOM	1432	CG1	ILE	B	69	55.861	53.307	5.925	1.00	17.84
ATOM	1433	CG2	ILE	B	69	57.274	52.750	7.990	1.00	14.87
ATOM	1434	CD1	ILE	B	69	54.757	52.283	6.267	1.00	16.76
ATOM	1435	N	SER	B	70	55.833	55.293	10.427	1.00	16.82
ATOM	1436	CA	SER	B	70	56.501	55.939	11.600	1.00	16.67
ATOM	1437	C	SER	B	70	56.965	54.905	12.627	1.00	16.91
ATOM	1438	O	SER	B	70	56.147	54.102	13.128	1.00	17.58
ATOM	1439	CB	SER	B	70	55.507	56.879	12.249	1.00	19.85
ATOM	1440	OG	SER	B	70	56.106	57.626	13.304	1.00	22.39
ATOM	1441	N	VAL	B	71	58.251	54.930	12.921	1.00	16.01
ATOM	1442	CA	VAL	B	71	58.827	53.962	13.933	1.00	17.80
ATOM	1443	C	VAL	B	71	58.832	54.719	15.270	1.00	22.32
ATOM	1444	O	VAL	B	71	59.512	55.723	15.417	1.00	23.49
ATOM	1445	CB	VAL	B	71	60.163	53.404	13.523	1.00	22.83
ATOM	1446	CG1	VAL	B	71	59.967	52.567	12.214	1.00	21.98
ATOM	1447	CG2	VAL	B	71	61.222	54.501	13.387	1.00	24.06
ATOM	1448	N	ASN	B	72	58.010	54.232	16.202	1.00	20.48
ATOM	1449	CA	ASN	B	72	57.806	54.878	17.519	1.00	20.13
ATOM	1450	C	ASN	B	72	58.320	54.086	18.687	1.00	22.39
ATOM	1451	O	ASN	B	72	58.488	52.863	18.621	1.00	22.18
ATOM	1452	CB	ASN	B	72	56.296	55.038	17.753	1.00	21.77
ATOM	1453	CG	ASN	B	72	55.591	55.775	16.621	1.00	30.59
ATOM	1454	OD1	ASN	B	72	56.228	56.530	15.869	1.00	25.69
ATOM	1455	ND2	ASN	B	72	54.279	55.529	16.469	1.00	26.90
ATOM	1456	N	GLY	B	73	58.520	54.790	19.792	1.00	20.53
ATOM	1457	CA	GLY	B	73	58.998	54.092	20.992	1.00	19.66
ATOM	1458	C	GLY	B	73	60.428	53.605	20.792	1.00	20.18
ATOM	1459	O	GLY	B	73	61.239	54.232	20.080	1.00	19.03
ATOM	1460	N	ALA	B	74	60.758	52.473	21.443	1.00	16.73

ATOM	1461	CA	ALA	B	74	62.107	51.908	21.352	1.00	16.27
ATOM	1462	C	ALA	B	74	62.580	51.614	19.912	1.00	17.37
ATOM	1463	O	ALA	B	74	63.776	51.649	19.637	1.00	18.06
ATOM	1464	CB	ALA	B	74	62.278	50.633	22.256	1.00	17.59
ATOM	1465	N	ALA	B	75	61.592	51.305	19.057	1.00	17.95
ATOM	1466	CA	ALA	B	75	61.873	50.961	17.639	1.00	17.42
ATOM	1467	C	ALA	B	75	62.567	52.115	16.916	1.00	19.91
ATOM	1468	O	ALA	B	75	63.215	51.889	15.889	1.00	19.81
ATOM	1469	CB	ALA	B	75	60.630	50.577	16.959	1.00	18.30
ATOM	1470	N	ALA	B	76	62.467	53.348	17.441	1.00	16.78
ATOM	1471	CA	ALA	B	76	63.152	54.470	16.804	1.00	18.31
ATOM	1472	C	ALA	B	76	64.688	54.276	16.795	1.00	18.92
ATOM	1473	O	ALA	B	76	65.409	54.921	16.046	1.00	19.50
ATOM	1474	CB	ALA	B	76	62.747	55.786	17.477	1.00	19.95
ATOM	1475	N	HIS	B	77	65.225	53.369	17.637	1.00	16.41
ATOM	1476	CA	HIS	B	77	66.629	53.103	17.671	1.00	17.43
ATOM	1477	C	HIS	B	77	67.082	52.158	16.543	1.00	18.10
ATOM	1478	O	HIS	B	77	68.280	51.967	16.351	1.00	20.06
ATOM	1479	CB	HIS	B	77	66.975	52.307	18.995	1.00	19.37
ATOM	1480	CG	HIS	B	77	67.026	53.149	20.241	1.00	22.65
ATOM	1481	ND1	HIS	B	77	68.174	53.787	20.649	1.00	25.27
ATOM	1482	CD2	HIS	B	77	66.090	53.421	21.181	1.00	22.98
ATOM	1483	CE1	HIS	B	77	67.944	54.431	21.784	1.00	24.52
ATOM	1484	NE2	HIS	B	77	66.688	54.230	22.129	1.00	23.17
ATOM	1485	N	CYS	B	78	66.107	51.548	15.846	1.00	17.70
ATOM	1486	CA	CYS	B	78	66.400	50.536	14.812	1.00	18.05
ATOM	1487	C	CYS	B	78	66.195	50.986	13.386	1.00	21.51
ATOM	1488	O	CYS	B	78	66.497	50.233	12.465	1.00	21.14
ATOM	1489	CB	CYS	B	78	65.489	49.332	15.033	1.00	19.61
ATOM	1490	SG	CYS	B	78	65.663	48.553	16.688	1.00	25.07
ATOM	1491	N	ALA	B	79	65.673	52.190	13.200	1.00	20.09
ATOM	1492	CA	ALA	B	79	65.471	52.690	11.843	1.00	19.73
ATOM	1493	C	ALA	B	79	65.477	54.201	11.864	1.00	25.47
ATOM	1494	O	ALA	B	79	65.094	54.811	12.852	1.00	23.97
ATOM	1495	CB	ALA	B	79	64.173	52.190	11.274	1.00	20.06
ATOM	1496	N	SER	B	80	65.895	54.802	10.750	1.00	21.56
ATOM	1497	CA	SER	B	80	65.935	56.270	10.595	1.00	22.17
ATOM	1498	C	SER	B	80	65.082	56.677	9.407	1.00	23.37
ATOM	1499	O	SER	B	80	64.831	55.862	8.511	1.00	21.62
ATOM	1500	CB	SER	B	80	67.335	56.763	10.301	1.00	25.03
ATOM	1501	OG	SER	B	80	68.302	56.327	11.243	1.00	28.26
ATOM	1502	N	VAL	B	81	64.652	57.936	9.398	1.00	18.88
ATOM	1503	CA	VAL	B	81	63.839	58.463	8.295	1.00	19.13
ATOM	1504	C	VAL	B	81	64.647	58.216	7.017	1.00	21.75
ATOM	1505	O	VAL	B	81	65.878	58.452	6.967	1.00	20.90
ATOM	1506	CB	VAL	B	81	63.576	59.970	8.514	1.00	21.73
ATOM	1507	CG1	VAL	B	81	63.015	60.599	7.224	1.00	22.57
ATOM	1508	CG2	VAL	B	81	62.555	60.148	9.631	1.00	21.80
ATOM	1509	N	GLY	B	82	63.961	57.728	5.988	1.00	18.71
ATOM	1510	CA	GLY	B	82	64.654	57.428	4.731	1.00	18.70
ATOM	1511	C	GLY	B	82	65.071	55.972	4.552	1.00	22.87
ATOM	1512	O	GLY	B	82	65.361	55.545	3.448	1.00	22.78
ATOM	1513	N	ASP	B	83	65.157	55.182	5.641	1.00	16.66
ATOM	1514	CA	ASP	B	83	65.546	53.791	5.481	1.00	16.76
ATOM	1515	C	ASP	B	83	64.461	53.003	4.716	1.00	16.77
ATOM	1516	O	ASP	B	83	63.257	53.256	4.890	1.00	17.18
ATOM	1517	CB	ASP	B	83	65.668	53.149	6.878	1.00	18.79
ATOM	1518	CG	ASP	B	83	66.945	53.556	7.622	1.00	22.59
ATOM	1519	OD1	ASP	B	83	67.788	54.320	7.106	1.00	20.93
ATOM	1520	OD2	ASP	B	83	67.141	53.058	8.771	1.00	21.88

ATOM	1521	N	ILE	B	84	64.912	52.031	3.926	1.00	17.58
ATOM	1522	CA	ILE	B	84	63.979	51.167	3.183	1.00	17.77
ATOM	1523	C	ILE	B	84	63.804	49.904	4.035	1.00	17.52
ATOM	1524	O	ILE	B	84	64.819	49.318	4.435	1.00	16.51
ATOM	1525	CB	ILE	B	84	64.627	50.788	1.851	1.00	21.87
ATOM	1526	CG1	ILE	B	84	64.840	52.071	1.020	1.00	22.20
ATOM	1527	CG2	ILE	B	84	63.771	49.760	1.060	1.00	22.70
ATOM	1528	CD1	ILE	B	84	65.694	51.766	-0.225	1.00	27.68
ATOM	1529	N	VAL	B	85	62.549	49.558	4.289	1.00	16.68
ATOM	1530	CA	VAL	B	85	62.253	48.361	5.100	1.00	14.93
ATOM	1531	C	VAL	B	85	61.196	47.462	4.460	1.00	18.77
ATOM	1532	O	VAL	B	85	60.487	47.874	3.522	1.00	18.51
ATOM	1533	CB	VAL	B	85	61.774	48.796	6.520	1.00	15.49
ATOM	1534	CG1	VAL	B	85	62.754	49.740	7.159	1.00	16.44
ATOM	1535	CG2	VAL	B	85	60.456	49.420	6.480	1.00	14.40
ATOM	1536	N	ILE	B	86	61.088	46.220	4.979	1.00	14.77
ATOM	1537	CA	ILE	B	86	60.101	45.258	4.557	1.00	15.52
ATOM	1538	C	ILE	B	86	59.318	44.987	5.853	1.00	15.28
ATOM	1539	O	ILE	B	86	59.977	44.736	6.887	1.00	15.56
ATOM	1540	CB	ILE	B	86	60.708	43.982	4.000	1.00	18.22
ATOM	1541	CG1	ILE	B	86	61.392	44.270	2.628	1.00	19.52
ATOM	1542	CG2	ILE	B	86	59.635	42.934	3.810	1.00	18.36
ATOM	1543	CD1	ILE	B	86	62.446	43.260	2.291	1.00	25.25
ATOM	1544	N	ILE	B	87	58.027	45.119	5.832	1.00	11.80
ATOM	1545	CA	ILE	B	87	57.150	44.909	7.039	1.00	11.37
ATOM	1546	C	ILE	B	87	56.294	43.697	6.765	1.00	16.80
ATOM	1547	O	ILE	B	87	55.535	43.669	5.743	1.00	15.75
ATOM	1548	CB	ILE	B	87	56.290	46.133	7.310	1.00	14.04
ATOM	1549	CG1	ILE	B	87	57.201	47.385	7.461	1.00	14.68
ATOM	1550	CG2	ILE	B	87	55.352	45.915	8.585	1.00	16.46
ATOM	1551	CD1	ILE	B	87	56.479	48.706	7.825	1.00	16.93
ATOM	1552	N	ALA	B	88	56.344	42.673	7.625	1.00	13.54
ATOM	1553	CA	ALA	B	88	55.573	41.433	7.389	1.00	12.01
ATOM	1554	C	ALA	B	88	54.747	40.989	8.570	1.00	15.27
ATOM	1555	O	ALA	B	88	55.124	41.315	9.709	1.00	14.13
ATOM	1556	CB	ALA	B	88	56.578	40.310	7.103	1.00	12.68
ATOM	1557	N	SER	B	89	53.681	40.257	8.354	1.00	11.75
ATOM	1558	CA	SER	B	89	52.915	39.648	9.450	1.00	9.22
ATOM	1559	C	SER	B	89	52.832	38.161	9.095	1.00	13.85
ATOM	1560	O	SER	B	89	52.842	37.761	7.892	1.00	12.02
ATOM	1561	CB	SER	B	89	51.576	40.264	9.748	1.00	13.00
ATOM	1562	OG	SER	B	89	50.496	39.710	8.999	1.00	13.68
ATOM	1563	N	PHE	B	90	52.719	37.289	10.096	1.00	9.51
ATOM	1564	CA	PHE	B	90	52.623	35.844	9.949	1.00	10.69
ATOM	1565	C	PHE	B	90	51.374	35.318	10.617	1.00	14.12
ATOM	1566	O	PHE	B	90	50.966	35.838	11.662	1.00	13.43
ATOM	1567	CB	PHE	B	90	53.867	35.159	10.575	1.00	9.99
ATOM	1568	CG	PHE	B	90	55.113	35.353	9.734	1.00	8.63
ATOM	1569	CD1	PHE	B	90	55.859	36.535	9.814	1.00	12.75
ATOM	1570	CD2	PHE	B	90	55.522	34.331	8.843	1.00	9.84
ATOM	1571	CE1	PHE	B	90	57.025	36.701	9.041	1.00	12.66
ATOM	1572	CE2	PHE	B	90	56.641	34.530	8.034	1.00	11.34
ATOM	1573	CZ	PHE	B	90	57.402	35.653	8.117	1.00	11.79
ATOM	1574	N	VAL	B	91	50.758	34.290	10.053	1.00	11.04
ATOM	1575	CA	VAL	B	91	49.550	33.671	10.631	1.00	8.97
ATOM	1576	C	VAL	B	91	49.759	32.182	10.733	1.00	12.88
ATOM	1577	O	VAL	B	91	50.664	31.609	10.051	1.00	13.37
ATOM	1578	CB	VAL	B	91	48.248	33.943	9.847	1.00	11.62
ATOM	1579	CG1	VAL	B	91	47.808	35.362	9.981	1.00	11.91
ATOM	1580	CG2	VAL	B	91	48.467	33.557	8.297	1.00	13.43

ATOM	1581	N	THR	B	92	48.950	31.506	11.576	1.00	11.67
ATOM	1582	CA	THR	B	92	49.050	30.076	11.700	1.00	9.61
ATOM	1583	C	THR	B	92	47.768	29.379	11.153	1.00	8.31
ATOM	1584	O	THR	B	92	46.695	29.929	11.140	1.00	11.35
ATOM	1585	CB	THR	B	92	49.410	29.637	13.156	1.00	12.02
ATOM	1586	OG1	THR	B	92	48.375	30.148	14.048	1.00	17.42
ATOM	1587	CG2	THR	B	92	50.764	30.137	13.517	1.00	11.07
ATOM	1588	N	MET	B	93	47.931	28.135	10.727	1.00	10.31
ATOM	1589	CA	MET	B	93	46.813	27.363	10.119	1.00	10.55
ATOM	1590	C	MET	B	93	47.283	25.922	9.940	1.00	10.55
ATOM	1591	O	MET	B	93	48.489	25.635	9.886	1.00	11.69
ATOM	1592	CB	MET	B	93	46.433	27.950	8.677	1.00	11.27
ATOM	1593	CG	MET	B	93	47.606	27.775	7.732	1.00	11.07
ATOM	1594	SD	MET	B	93	47.367	28.740	6.145	1.00	13.35
ATOM	1595	CE	MET	B	93	47.673	30.365	6.821	1.00	13.30
ATOM	1596	N	PRO	B	94	46.310	25.017	9.819	1.00	10.89
ATOM	1597	CA	PRO	B	94	46.643	23.597	9.614	1.00	10.92
ATOM	1598	C	PRO	B	94	47.476	23.350	8.341	1.00	13.89
ATOM	1599	O	PRO	B	94	47.320	24.098	7.342	1.00	13.64
ATOM	1600	CB	PRO	B	94	45.279	22.924	9.495	1.00	15.15
ATOM	1601	CG	PRO	B	94	44.323	23.877	10.157	1.00	18.73
ATOM	1602	CD	PRO	B	94	44.883	25.258	9.963	1.00	13.59
ATOM	1603	N	ASP	B	95	48.342	22.360	8.373	1.00	12.77
ATOM	1604	CA	ASP	B	95	49.212	22.008	7.262	1.00	11.85
ATOM	1605	C	ASP	B	95	48.393	21.914	5.939	1.00	12.73
ATOM	1606	O	ASP	B	95	48.870	22.437	4.868	1.00	14.23
ATOM	1607	CB	ASP	B	95	49.866	20.644	7.529	1.00	13.88
ATOM	1608	CG	ASP	B	95	50.845	20.258	6.464	1.00	16.93
ATOM	1609	OD1	ASP	B	95	51.845	20.951	6.229	1.00	15.12
ATOM	1610	OD2	ASP	B	95	50.556	19.245	5.782	1.00	25.27
ATOM	1611	N	GLU	B	96	47.243	21.265	6.009	1.00	11.92
ATOM	1612	CA	GLU	B	96	46.390	21.080	4.780	1.00	13.09
ATOM	1613	C	GLU	B	96	46.038	22.401	4.116	1.00	17.50
ATOM	1614	O	GLU	B	96	46.007	22.470	2.870	1.00	17.59
ATOM	1615	CB	GLU	B	96	45.127	20.359	5.163	1.00	15.73
ATOM	1616	CG	GLU	B	96	44.284	19.936	3.967	1.00	27.44
ATOM	1617	CD	GLU	B	96	43.202	20.920	3.636	1.00	46.48
ATOM	1618	OE1	GLU	B	96	42.841	21.740	4.488	1.00	32.53
ATOM	1619	OE2	GLU	B	96	42.694	20.865	2.486	1.00	50.29
ATOM	1620	N	GLU	B	97	45.759	23.446	4.888	1.00	13.12
ATOM	1621	CA	GLU	B	97	45.427	24.755	4.311	1.00	11.58
ATOM	1622	C	GLU	B	97	46.740	25.459	3.880	1.00	14.13
ATOM	1623	O	GLU	B	97	46.819	26.229	2.912	1.00	14.05
ATOM	1624	CB	GLU	B	97	44.687	25.646	5.357	1.00	10.79
ATOM	1625	CG	GLU	B	97	43.358	25.155	5.736	1.00	12.84
ATOM	1626	CD	GLU	B	97	42.625	26.039	6.749	1.00	16.10
ATOM	1627	OE1	GLU	B	97	43.205	27.015	7.351	1.00	17.56
ATOM	1628	OE2	GLU	B	97	41.424	25.785	6.889	1.00	19.58
ATOM	1629	N	ALA	B	98	47.825	25.307	4.639	1.00	11.26
ATOM	1630	CA	ALA	B	98	49.073	25.952	4.345	1.00	12.13
ATOM	1631	C	ALA	B	98	49.676	25.620	2.956	1.00	12.78
ATOM	1632	O	ALA	B	98	50.385	26.476	2.363	1.00	12.87
ATOM	1633	CB	ALA	B	98	50.090	25.538	5.483	1.00	13.93
ATOM	1634	N	ARG	B	99	49.379	24.371	2.518	1.00	13.12
ATOM	1635	CA	ARG	B	99	49.910	23.918	1.252	1.00	13.91
ATOM	1636	C	ARG	B	99	49.405	24.782	0.094	1.00	15.52
ATOM	1637	O	ARG	B	99	50.124	24.819	-0.929	1.00	16.74
ATOM	1638	CB	ARG	B	99	49.565	22.459	1.069	1.00	13.81
ATOM	1639	CG	ARG	B	99	50.400	21.628	2.049	1.00	21.54
ATOM	1640	CD	ARG	B	99	50.114	20.193	2.018	1.00	31.31

ATOM	1641	NE	ARG	B	99	50.922	19.539	3.049	1.00	34.14
ATOM	1642	CZ	ARG	B	99	52.233	19.293	2.966	1.00	39.78
ATOM	1643	NH1	ARG	B	99	52.927	19.613	1.874	1.00	39.29
ATOM	1644	NH2	ARG	B	99	52.860	18.698	3.965	1.00	34.68
ATOM	1645	N	THR	B	100	48.273	25.465	0.233	1.00	12.99
ATOM	1646	CA	THR	B	100	47.765	26.311	-0.888	1.00	13.08
ATOM	1647	C	THR	B	100	47.681	27.801	-0.521	1.00	15.62
ATOM	1648	O	THR	B	100	47.191	28.652	-1.282	1.00	16.66
ATOM	1649	CB	THR	B	100	46.391	25.798	-1.313	1.00	15.79
ATOM	1650	OG1	THR	B	100	45.503	25.711	-0.202	1.00	14.58
ATOM	1651	CG2	THR	B	100	46.501	24.357	-1.922	1.00	15.05
ATOM	1652	N	TRP	B	101	48.179	28.176	0.681	1.00	14.25
ATOM	1653	CA	TRP	B	101	48.083	29.565	1.087	1.00	13.12
ATOM	1654	C	TRP	B	101	48.843	30.513	0.232	1.00	15.17
ATOM	1655	O	TRP	B	101	49.947	30.182	-0.256	1.00	16.82
ATOM	1656	CB	TRP	B	101	48.617	29.632	2.595	1.00	11.79
ATOM	1657	CG	TRP	B	101	48.657	31.026	3.110	1.00	10.50
ATOM	1658	CD1	TRP	B	101	49.734	31.812	3.259	1.00	12.40
ATOM	1659	CD2	TRP	B	101	47.519	31.822	3.403	1.00	12.89
ATOM	1660	NE1	TRP	B	101	49.344	33.048	3.665	1.00	12.65
ATOM	1661	CE2	TRP	B	101	47.998	33.095	3.786	1.00	13.88
ATOM	1662	CE3	TRP	B	101	46.141	31.580	3.424	1.00	15.74
ATOM	1663	CZ2	TRP	B	101	47.158	34.140	4.162	1.00	16.20
ATOM	1664	CZ3	TRP	B	101	45.272	32.635	3.777	1.00	19.25
ATOM	1665	CH2	TRP	B	101	45.792	33.914	4.137	1.00	19.62
ATOM	1666	N	ARG	B	102	48.283	31.722	0.072	1.00	15.08
ATOM	1667	CA	ARG	B	102	48.934	32.768	-0.695	1.00	15.90
ATOM	1668	C	ARG	B	102	48.968	34.063	0.149	1.00	11.33
ATOM	1669	O	ARG	B	102	47.928	34.506	0.584	1.00	14.41
ATOM	1670	CB	ARG	B	102	48.114	33.078	-1.993	1.00	18.89
ATOM	1671	CG	ARG	B	102	48.011	31.878	-2.994	1.00	24.40
ATOM	1672	CD	ARG	B	102	47.276	32.241	-4.310	1.00	22.77
ATOM	1673	NE	ARG	B	102	47.968	33.268	-5.060	1.00	27.18
ATOM	1674	CZ	ARG	B	102	48.980	33.060	-5.903	1.00	28.35
ATOM	1675	NH1	ARG	B	102	49.464	31.849	-6.107	1.00	23.60
ATOM	1676	NH2	ARG	B	102	49.523	34.086	-6.528	1.00	31.92
ATOM	1677	N	PRO	B	103	50.154	34.655	0.289	1.00	12.26
ATOM	1678	CA	PRO	B	103	50.259	35.917	1.065	1.00	13.54
ATOM	1679	C	PRO	B	103	49.796	37.123	0.286	1.00	17.32
ATOM	1680	O	PRO	B	103	49.731	37.056	-1.006	1.00	16.83
ATOM	1681	CB	PRO	B	103	51.763	36.065	1.280	1.00	14.38
ATOM	1682	CG	PRO	B	103	52.386	35.452	0.019	1.00	22.25
ATOM	1683	CD	PRO	B	103	51.461	34.218	-0.225	1.00	16.38
ATOM	1684	N	ASN	B	104	49.507	38.228	1.005	1.00	13.82
ATOM	1685	CA	ASN	B	104	49.083	39.495	0.409	1.00	12.48
ATOM	1686	C	ASN	B	104	50.317	40.372	0.282	1.00	19.52
ATOM	1687	O	ASN	B	104	50.868	40.809	1.326	1.00	16.91
ATOM	1688	CB	ASN	B	104	48.000	40.183	1.247	1.00	13.72
ATOM	1689	CG	ASN	B	104	46.823	39.329	1.441	1.00	19.91
ATOM	1690	OD1	ASN	B	104	46.218	38.875	0.448	1.00	17.05
ATOM	1691	ND2	ASN	B	104	46.460	39.032	2.699	1.00	20.70
ATOM	1692	N	VAL	B	105	50.789	40.668	-0.936	1.00	17.67
ATOM	1693	CA	VAL	B	105	51.984	41.447	-1.064	1.00	16.36
ATOM	1694	C	VAL	B	105	51.762	42.755	-1.760	1.00	21.93
ATOM	1695	O	VAL	B	105	51.102	42.783	-2.816	1.00	22.45
ATOM	1696	CB	VAL	B	105	53.090	40.681	-1.848	1.00	18.76
ATOM	1697	CG1	VAL	B	105	54.343	41.495	-1.957	1.00	19.86
ATOM	1698	CG2	VAL	B	105	53.336	39.231	-1.253	1.00	19.00
ATOM	1699	N	ALA	B	106	52.287	43.832	-1.188	1.00	20.08
ATOM	1700	CA	ALA	B	106	52.199	45.188	-1.794	1.00	19.28

ATOM	1701	C	ALA	B	106	53.617	45.637	-2.080	1.00	22.54
ATOM	1702	O	ALA	B	106	54.491	45.558	-1.214	1.00	20.02
ATOM	1703	CB	ALA	B	106	51.533	46.151	-0.903	1.00	19.59
ATOM	1704	N	TYR	B	107	53.895	46.128	-3.312	1.00	21.77
ATOM	1705	CA	TYR	B	107	55.244	46.571	-3.683	1.00	22.90
ATOM	1706	C	TYR	B	107	55.292	48.084	-3.760	1.00	25.98
ATOM	1707	O	TYR	B	107	54.300	48.712	-4.096	1.00	25.22
ATOM	1708	CB	TYR	B	107	55.668	45.972	-5.032	1.00	25.00
ATOM	1709	CG	TYR	B	107	55.904	44.492	-4.966	1.00	24.25
ATOM	1710	CD1	TYR	B	107	57.129	43.980	-4.544	1.00	26.30
ATOM	1711	CD2	TYR	B	107	54.888	43.600	-5.316	1.00	25.93
ATOM	1712	CE1	TYR	B	107	57.342	42.629	-4.484	1.00	29.13
ATOM	1713	CE2	TYR	B	107	55.100	42.234	-5.270	1.00	25.26
ATOM	1714	CZ	TYR	B	107	56.326	41.757	-4.872	1.00	31.88
ATOM	1715	OH	TYR	B	107	56.524	40.388	-4.808	1.00	35.96
ATOM	1716	N	PHE	B	108	56.446	48.652	-3.408	1.00	26.53
ATOM	1717	CA	PHE	B	108	56.584	50.098	-3.399	1.00	25.71
ATOM	1718	C	PHE	B	108	57.894	50.568	-4.005	1.00	31.22
ATOM	1719	O	PHE	B	108	58.893	49.844	-4.074	1.00	28.62
ATOM	1720	CB	PHE	B	108	56.572	50.645	-1.933	1.00	25.29
ATOM	1721	CG	PHE	B	108	55.293	50.411	-1.188	1.00	21.78
ATOM	1722	CD1	PHE	B	108	55.033	49.174	-0.571	1.00	19.05
ATOM	1723	CD2	PHE	B	108	54.354	51.421	-1.064	1.00	20.20
ATOM	1724	CE1	PHE	B	108	53.856	48.967	0.111	1.00	19.07
ATOM	1725	CE2	PHE	B	108	53.187	51.237	-0.377	1.00	22.77
ATOM	1726	CZ	PHE	B	108	52.950	49.952	0.240	1.00	20.24
ATOM	1727	N	GLU	B	109	57.864	51.828	-4.412	1.00	30.97
ATOM	1728	CA	GLU	B	109	59.012	52.499	-5.011	1.00	32.90
ATOM	1729	C	GLU	B	109	58.921	53.977	-4.680	1.00	33.93
ATOM	1730	O	GLU	B	109	57.889	54.468	-4.269	1.00	30.42
ATOM	1731	CB	GLU	B	109	58.916	52.388	-6.540	1.00	35.17
ATOM	1732	CG	GLU	B	109	57.721	53.172	-7.089	1.00	44.89
ATOM	1733	CD	GLU	B	109	57.496	52.955	-8.566	1.00	68.70
ATOM	1734	OE1	GLU	B	109	58.416	52.425	-9.234	1.00	58.38
ATOM	1735	OE2	GLU	B	109	56.391	53.305	-9.056	1.00	66.11
ATOM	1736	N	GLY	B	110	60.008	54.705	-4.916	1.00	33.06
ATOM	1737	CA	GLY	B	110	60.007	56.135	-4.668	1.00	32.35
ATOM	1738	C	GLY	B	110	59.545	56.486	-3.270	1.00	35.50
ATOM	1739	O	GLY	B	110	60.045	55.920	-2.286	1.00	35.53
ATOM	1740	N	ASP	B	111	58.646	57.449	-3.185	1.00	29.97
ATOM	1741	CA	ASP	B	111	58.151	57.917	-1.907	1.00	31.05
ATOM	1742	C	ASP	B	111	56.884	57.180	-1.499	1.00	30.82
ATOM	1743	O	ASP	B	111	55.761	57.743	-1.439	1.00	28.67
ATOM	1744	CB	ASP	B	111	57.984	59.438	-1.931	1.00	33.49
ATOM	1745	CG	ASP	B	111	57.207	59.966	-0.755	1.00	44.31
ATOM	1746	OD1	ASP	B	111	57.431	59.473	0.386	1.00	46.12
ATOM	1747	OD2	ASP	B	111	56.359	60.857	-0.974	1.00	41.60
ATOM	1748	N	ASN	B	112	57.084	55.909	-1.181	1.00	27.75
ATOM	1749	CA	ASN	B	112	55.987	55.068	-0.770	1.00	25.85
ATOM	1750	C	ASN	B	112	54.870	55.008	-1.770	1.00	28.56
ATOM	1751	O	ASN	B	112	53.695	55.087	-1.425	1.00	24.07
ATOM	1752	CB	ASN	B	112	55.512	55.413	0.637	1.00	25.14
ATOM	1753	CG	ASN	B	112	56.544	55.084	1.628	1.00	19.48
ATOM	1754	OD1	ASN	B	112	57.512	54.410	1.275	1.00	22.70
ATOM	1755	ND2	ASN	B	112	56.399	55.582	2.868	1.00	21.36
ATOM	1756	N	GLU	B	113	55.271	54.857	-3.032	1.00	27.11
ATOM	1757	CA	GLU	B	113	54.288	54.748	-4.114	1.00	28.84
ATOM	1758	C	GLU	B	113	54.071	53.286	-4.361	1.00	27.72
ATOM	1759	O	GLU	B	113	55.024	52.572	-4.769	1.00	26.82
ATOM	1760	CB	GLU	B	113	54.752	55.441	-5.391	1.00	30.87

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ATOM   1761  CG  GLU B 113      54.797  56.958  -5.306  1.00 37.93
ATOM   1762  CD  GLU B 113      53.442  57.703  -5.230  1.00 59.74
ATOM   1763  OE1 GLU B 113      52.345  57.089  -5.096  1.00 46.50
ATOM   1764  OE2 GLU B 113      53.517  58.956  -5.296  1.00 59.60
ATOM   1765  N   MET B 114      52.842  52.856  -4.080  1.00 27.25
ATOM   1766  CA  MET B 114      52.436  51.459  -4.226  1.00 32.32
ATOM   1767  C   MET B 114      52.272  51.103  -5.666  1.00 39.86
ATOM   1768  O   MET B 114      51.463  51.727  -6.359  1.00 40.94
ATOM   1769  CB  MET B 114      51.094  51.203  -3.533  1.00 34.33
ATOM   1770  CG  MET B 114      50.808  49.728  -3.412  1.00 36.77
ATOM   1771  SD  MET B 114      49.151  49.352  -2.940  1.00 39.76
ATOM   1772  CE  MET B 114      49.252  49.698  -1.017  1.00 31.31
ATOM   1773  N   LYS B 115      53.006  50.104  -6.129  1.00 37.37
ATOM   1774  CA  LYS B 115      52.918  49.687  -7.538  1.00 38.95
ATOM   1775  C   LYS B 115      51.644  48.899  -7.836  1.00 54.19
ATOM   1776  O   LYS B 115      51.157  48.178  -6.919  1.00 51.66
ATOM   1777  CB  LYS B 115      54.114  48.851  -7.929  1.00 41.43
ATOM   1778  CG  LYS B 115      55.452  49.572  -7.954  1.00 47.27
ATOM   1779  CD  LYS B 115      56.543  48.571  -8.255  1.00 43.78
ATOM   1780  CE  LYS B 115      57.915  49.055  -7.874  1.00 55.99
ATOM   1781  NZ  LYS B 115      58.975  48.255  -8.577  1.00 62.59
ATOM      1  N   MET C   1      48.433  20.814  26.350  1.00 25.25
ATOM      2  CA  MET C   1      49.028  22.003  25.752  1.00 23.37
ATOM      3  C   MET C   1      49.715  21.688  24.462  1.00 22.04
ATOM      4  O   MET C   1      49.875  20.523  24.092  1.00 22.16
ATOM      5  CB  MET C   1      49.850  22.851  26.665  1.00 26.58
ATOM      6  CG  MET C   1      50.670  22.110  27.510  1.00 29.48
ATOM      7  SD  MET C   1      51.965  21.246  26.703  1.00 32.96
ATOM      8  CE  MET C   1      52.813  20.920  28.227  1.00 23.68
ATOM      9  N   ILE C   2      50.100  22.747  23.803  1.00 14.33
ATOM     10  CA  ILE C   2      50.686  22.664  22.441  1.00 12.86
ATOM     11  C   ILE C   2      52.160  22.979  22.400  1.00 13.27
ATOM     12  O   ILE C   2      52.627  24.031  22.948  1.00 12.60
ATOM     13  CB  ILE C   2      49.882  23.673  21.576  1.00 15.76
ATOM     14  CG1 ILE C   2      48.390  23.281  21.509  1.00 18.95
ATOM     15  CG2 ILE C   2      50.477  23.802  20.155  1.00 15.91
ATOM     16  CD1 ILE C   2      48.150  22.002  20.809  1.00 30.84
ATOM     17  N   ARG C   3      52.927  22.092  21.751  1.00 11.28
ATOM     18  CA  ARG C   3      54.380  22.286  21.644  1.00 10.27
ATOM     19  C   ARG C   3      54.824  22.880  20.295  1.00 12.97
ATOM     20  O   ARG C   3      54.091  22.691  19.313  1.00 11.98
ATOM     21  CB  ARG C   3      55.085  20.920  21.683  1.00 11.24
ATOM     22  CG  ARG C   3      54.887  20.123  23.057  1.00 11.07
ATOM     23  CD  ARG C   3      55.885  20.640  24.091  1.00 14.19
ATOM     24  NE  ARG C   3      55.755  19.688  25.224  1.00 12.85
ATOM     25  CZ  ARG C   3      56.624  19.664  26.235  1.00 13.01
ATOM     26  NH1 ARG C   3      57.564  20.552  26.371  1.00 11.87
ATOM     27  NH2 ARG C   3      56.424  18.698  27.173  1.00 15.42
ATOM     28  N   THR C   4      55.967  23.542  20.295  1.00 10.90
ATOM     29  CA  THR C   4      56.599  24.104  19.048  1.00  8.73
ATOM     30  C   THR C   4      57.765  23.120  18.793  1.00 12.54
ATOM     31  O   THR C   4      58.739  23.023  19.649  1.00 11.96
ATOM     32  CB  THR C   4      57.080  25.498  19.237  1.00 10.20
ATOM     33  OG1 THR C   4      55.949  26.331  19.490  1.00 12.29
ATOM     34  CG2 THR C   4      57.908  26.008  17.930  1.00 12.13
ATOM     35  N   MET C   5      57.701  22.369  17.637  1.00 10.12
ATOM     36  CA  MET C   5      58.676  21.370  17.349  1.00 10.31
ATOM     37  C   MET C   5      59.356  21.600  16.015  1.00 13.52
ATOM     38  O   MET C   5      58.720  22.172  15.112  1.00 14.15
ATOM     39  CB  MET C   5      57.978  20.006  17.214  1.00 13.06
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ATOM	40	CG	MET	C	5	57.123	19.561	18.416	1.00	11.30
ATOM	41	SD	MET	C	5	58.165	19.333	19.918	1.00	13.37
ATOM	42	CE	MET	C	5	59.104	17.873	19.482	1.00	14.97
ATOM	43	N	LEU	C	6	60.600	21.155	15.915	1.00	10.44
ATOM	44	CA	LEU	C	6	61.345	21.255	14.605	1.00	11.49
ATOM	45	C	LEU	C	6	60.559	20.378	13.639	1.00	13.65
ATOM	46	O	LEU	C	6	60.436	19.139	13.800	1.00	12.95
ATOM	47	CB	LEU	C	6	62.722	20.660	14.786	1.00	11.43
ATOM	48	CG	LEU	C	6	63.587	20.673	13.484	1.00	12.67
ATOM	49	CD1	LEU	C	6	64.038	22.096	13.201	1.00	13.37
ATOM	50	CD2	LEU	C	6	64.839	19.829	13.742	1.00	14.36
ATOM	51	N	GLN	C	7	60.049	21.016	12.552	1.00	12.16
ATOM	52	CA	GLN	C	7	59.313	20.301	11.511	1.00	11.30
ATOM	53	C	GLN	C	7	60.333	19.599	10.566	1.00	12.23
ATOM	54	O	GLN	C	7	60.125	18.449	10.136	1.00	11.94
ATOM	55	CB	GLN	C	7	58.544	21.330	10.679	1.00	12.62
ATOM	56	CG	GLN	C	7	57.590	20.710	9.638	1.00	14.99
ATOM	57	CD	GLN	C	7	58.349	20.221	8.351	1.00	12.25
ATOM	58	OE1	GLN	C	7	58.036	19.083	7.865	1.00	14.42
ATOM	59	NE2	GLN	C	7	59.299	21.005	7.831	1.00	13.59
ATOM	60	N	GLY	C	8	61.406	20.329	10.295	1.00	12.10
ATOM	61	CA	GLY	C	8	62.459	19.795	9.406	1.00	12.14
ATOM	62	C	GLY	C	8	63.526	20.838	9.181	1.00	11.21
ATOM	63	O	GLY	C	8	63.403	22.022	9.565	1.00	12.25
ATOM	64	N	LYS	C	9	64.617	20.409	8.526	1.00	11.80
ATOM	65	CA	LYS	C	9	65.690	21.351	8.271	1.00	12.75
ATOM	66	C	LYS	C	9	66.604	20.908	7.117	1.00	12.69
ATOM	67	O	LYS	C	9	66.658	19.711	6.780	1.00	14.09
ATOM	68	CB	LYS	C	9	66.597	21.557	9.528	1.00	16.31
ATOM	69	CG	LYS	C	9	67.451	20.367	9.927	1.00	16.10
ATOM	70	CD	LYS	C	9	68.486	20.654	11.059	1.00	15.95
ATOM	71	CE	LYS	C	9	69.247	19.377	11.363	1.00	20.48
ATOM	72	NZ	LYS	C	9	70.409	19.689	12.260	1.00	22.05
ATOM	73	N	LEU	C	10	67.301	21.896	6.578	1.00	13.44
ATOM	74	CA	LEU	C	10	68.300	21.680	5.503	1.00	13.72
ATOM	75	C	LEU	C	10	69.586	21.951	6.258	1.00	14.03
ATOM	76	O	LEU	C	10	69.859	23.078	6.661	1.00	15.46
ATOM	77	CB	LEU	C	10	68.111	22.719	4.364	1.00	13.59
ATOM	78	CG	LEU	C	10	66.761	22.626	3.674	1.00	14.77
ATOM	79	CD1	LEU	C	10	66.548	23.780	2.652	1.00	18.67
ATOM	80	CD2	LEU	C	10	66.545	21.240	2.957	1.00	15.75
ATOM	81	N	HIS	C	11	70.365	20.925	6.451	1.00	14.06
ATOM	82	CA	HIS	C	11	71.591	21.029	7.244	1.00	14.41
ATOM	83	C	HIS	C	11	72.871	21.241	6.448	1.00	18.20
ATOM	84	O	HIS	C	11	73.258	20.362	5.684	1.00	16.24
ATOM	85	CB	HIS	C	11	71.710	19.803	8.172	1.00	17.29
ATOM	86	CG	HIS	C	11	72.805	19.913	9.185	1.00	18.36
ATOM	87	ND1	HIS	C	11	72.634	20.553	10.405	1.00	20.19
ATOM	88	CD2	HIS	C	11	74.087	19.464	9.174	1.00	19.36
ATOM	89	CE1	HIS	C	11	73.769	20.514	11.075	1.00	19.59
ATOM	90	NE2	HIS	C	11	74.667	19.854	10.354	1.00	18.93
ATOM	91	N	ARG	C	12	73.488	22.401	6.662	1.00	15.16
ATOM	92	CA	ARG	C	12	74.713	22.792	6.029	1.00	15.13
ATOM	93	C	ARG	C	12	74.613	22.974	4.525	1.00	16.37
ATOM	94	O	ARG	C	12	75.468	22.446	3.763	1.00	18.19
ATOM	95	CB	ARG	C	12	75.855	21.874	6.378	1.00	15.43
ATOM	96	CG	ARG	C	12	76.247	21.969	7.868	1.00	17.33
ATOM	97	CD	ARG	C	12	77.390	21.001	8.248	1.00	17.26
ATOM	98	NE	ARG	C	12	78.587	21.294	7.454	1.00	19.17
ATOM	99	CZ	ARG	C	12	79.529	22.164	7.760	1.00	24.65

ATOM	100	NH1	ARG	C	12	79.495	22.858	8.879	1.00	21.82
ATOM	101	NH2	ARG	C	12	80.545	22.350	6.912	1.00	28.03
ATOM	102	N	VAL	C	13	73.610	23.681	4.119	1.00	15.70
ATOM	103	CA	VAL	C	13	73.518	23.999	2.680	1.00	14.78
ATOM	104	C	VAL	C	13	74.416	25.241	2.524	1.00	18.42
ATOM	105	O	VAL	C	13	74.709	26.004	3.506	1.00	15.58
ATOM	106	CB	VAL	C	13	72.143	24.332	2.183	1.00	16.79
ATOM	107	CG1	VAL	C	13	71.318	23.094	2.020	1.00	18.88
ATOM	108	CG2	VAL	C	13	71.441	25.456	3.067	1.00	16.41
ATOM	109	N	LYS	C	14	74.877	25.500	1.273	1.00	15.68
ATOM	110	CA	LYS	C	14	75.726	26.646	0.997	1.00	16.45
ATOM	111	C	LYS	C	14	74.946	27.738	0.258	1.00	16.56
ATOM	112	O	LYS	C	14	74.116	27.432	-0.670	1.00	16.75
ATOM	113	CB	LYS	C	14	76.910	26.216	0.127	1.00	17.97
ATOM	114	CG	LYS	C	14	77.913	27.344	-0.094	1.00	20.97
ATOM	115	CD	LYS	C	14	79.173	26.878	-0.788	1.00	29.18
ATOM	116	CE	LYS	C	14	80.063	26.092	0.120	1.00	32.48
ATOM	117	NZ	LYS	C	14	81.181	25.545	-0.697	1.00	33.64
ATOM	118	N	VAL	C	15	75.161	29.013	0.665	1.00	13.79
ATOM	119	CA	VAL	C	15	74.467	30.142	0.040	1.00	14.02
ATOM	120	C	VAL	C	15	75.067	30.312	-1.393	1.00	14.49
ATOM	121	O	VAL	C	15	76.279	30.376	-1.536	1.00	14.91
ATOM	122	CB	VAL	C	15	74.678	31.451	0.826	1.00	14.72
ATOM	123	CG1	VAL	C	15	74.032	32.595	0.091	1.00	15.47
ATOM	124	CG2	VAL	C	15	74.013	31.273	2.287	1.00	15.44
ATOM	125	N	THR	C	16	74.182	30.292	-2.386	1.00	14.68
ATOM	126	CA	THR	C	16	74.627	30.393	-3.796	1.00	16.18
ATOM	127	C	THR	C	16	74.478	31.743	-4.444	1.00	19.63
ATOM	128	O	THR	C	16	75.143	31.995	-5.472	1.00	18.35
ATOM	129	CB	THR	C	16	73.869	29.362	-4.630	1.00	14.13
ATOM	130	OG1	THR	C	16	72.510	29.698	-4.778	1.00	17.95
ATOM	131	CG2	THR	C	16	74.103	27.943	-4.087	1.00	18.04
ATOM	132	N	HIS	C	17	73.636	32.604	-3.913	1.00	14.05
ATOM	133	CA	HIS	C	17	73.411	33.927	-4.456	1.00	15.34
ATOM	134	C	HIS	C	17	72.897	34.888	-3.343	1.00	19.86
ATOM	135	O	HIS	C	17	72.249	34.434	-2.351	1.00	17.90
ATOM	136	CB	HIS	C	17	72.332	33.779	-5.554	1.00	18.53
ATOM	137	CG	HIS	C	17	72.007	35.052	-6.293	1.00	22.33
ATOM	138	ND1	HIS	C	17	70.836	35.746	-6.083	1.00	25.17
ATOM	139	CD2	HIS	C	17	72.665	35.724	-7.285	1.00	24.77
ATOM	140	CE1	HIS	C	17	70.797	36.809	-6.865	1.00	25.62
ATOM	141	NE2	HIS	C	17	71.889	36.822	-7.610	1.00	24.55
ATOM	142	N	ALA	C	18	73.134	36.180	-3.515	1.00	16.82
ATOM	143	CA	ALA	C	18	72.649	37.211	-2.563	1.00	18.95
ATOM	144	C	ALA	C	18	72.073	38.366	-3.404	1.00	25.44
ATOM	145	O	ALA	C	18	72.647	38.737	-4.442	1.00	26.69
ATOM	146	CB	ALA	C	18	73.758	37.674	-1.645	1.00	21.19
ATOM	147	N	ASP	C	19	70.925	38.880	-3.029	1.00	21.26
ATOM	148	CA	ASP	C	19	70.290	39.955	-3.794	1.00	20.78
ATOM	149	C	ASP	C	19	69.612	40.957	-2.869	1.00	21.60
ATOM	150	O	ASP	C	19	68.413	40.890	-2.634	1.00	20.10
ATOM	151	CB	ASP	C	19	69.267	39.317	-4.767	1.00	21.77
ATOM	152	CG	ASP	C	19	68.692	40.307	-5.798	1.00	27.20
ATOM	153	OD1	ASP	C	19	69.092	41.478	-5.831	1.00	27.06
ATOM	154	OD2	ASP	C	19	67.785	39.862	-6.570	1.00	28.93
ATOM	155	N	LEU	C	20	70.393	41.917	-2.414	1.00	21.47
ATOM	156	CA	LEU	C	20	69.874	42.953	-1.551	1.00	21.15
ATOM	157	C	LEU	C	20	68.714	43.709	-2.138	1.00	25.20
ATOM	158	O	LEU	C	20	67.771	44.028	-1.426	1.00	24.39
ATOM	159	CB	LEU	C	20	70.997	43.944	-1.181	1.00	21.58

ATOM	160	CG	LEU	C	20	70.700	45.069	-0.209	1.00	24.50
ATOM	161	CD1	LEU	C	20	70.505	44.452	1.236	1.00	22.31
ATOM	162	CD2	LEU	C	20	71.937	46.004	-0.224	1.00	24.07
ATOM	163	N	HIS	C	21	68.786	44.010	-3.448	1.00	23.99
ATOM	164	CA	HIS	C	21	67.733	44.767	-4.147	1.00	26.08
ATOM	165	C	HIS	C	21	66.608	43.995	-4.713	1.00	29.17
ATOM	166	O	HIS	C	21	65.847	44.534	-5.516	1.00	29.91
ATOM	167	CB	HIS	C	21	68.393	45.692	-5.187	1.00	29.07
ATOM	168	CG	HIS	C	21	69.496	46.484	-4.609	1.00	34.17
ATOM	169	ND1	HIS	C	21	69.283	47.347	-3.561	1.00	37.06
ATOM	170	CD2	HIS	C	21	70.836	46.468	-4.819	1.00	37.54
ATOM	171	CE1	HIS	C	21	70.433	47.875	-3.181	1.00	36.64
ATOM	172	NE2	HIS	C	21	71.394	47.358	-3.926	1.00	37.19
ATOM	173	N	TYR	C	22	66.495	42.726	-4.309	1.00	26.33
ATOM	174	CA	TYR	C	22	65.413	41.864	-4.797	1.00	27.04
ATOM	175	C	TYR	C	22	64.087	42.615	-4.779	1.00	33.24
ATOM	176	O	TYR	C	22	63.709	43.265	-3.775	1.00	26.75
ATOM	177	CB	TYR	C	22	65.294	40.643	-3.890	1.00	28.34
ATOM	178	CG	TYR	C	22	64.348	39.561	-4.368	1.00	30.64
ATOM	179	CD1	TYR	C	22	64.555	38.917	-5.581	1.00	31.96
ATOM	180	CD2	TYR	C	22	63.290	39.162	-3.575	1.00	32.31
ATOM	181	CE1	TYR	C	22	63.697	37.898	-6.009	1.00	32.16
ATOM	182	CE2	TYR	C	22	62.421	38.161	-3.993	1.00	32.82
ATOM	183	CZ	TYR	C	22	62.641	37.525	-5.201	1.00	36.63
ATOM	184	OH	TYR	C	22	61.767	36.526	-5.622	1.00	38.85
ATOM	185	N	GLU	C	23	63.378	42.561	-5.883	1.00	34.58
ATOM	186	CA	GLU	C	23	62.134	43.254	-5.953	1.00	37.52
ATOM	187	C	GLU	C	23	60.863	42.459	-5.743	1.00	42.30
ATOM	188	O	GLU	C	23	59.798	43.013	-5.859	1.00	40.71
ATOM	189	CB	GLU	C	23	62.051	44.110	-7.214	1.00	39.74
ATOM	190	CG	GLU	C	23	63.078	45.231	-7.233	1.00	50.28
ATOM	191	CD	GLU	C	23	62.519	46.537	-6.691	1.00	61.64
ATOM	192	OE1	GLU	C	23	61.445	46.515	-6.046	1.00	62.40
ATOM	193	OE2	GLU	C	23	63.152	47.594	-6.923	1.00	61.54
ATOM	194	N	GLY	C	24	60.956	41.158	-5.438	1.00	39.86
ATOM	195	CA	GLY	C	24	59.736	40.345	-5.222	1.00	43.77
ATOM	196	C	GLY	C	24	59.575	39.938	-3.749	1.00	49.67
ATOM	197	O	GLY	C	24	58.617	39.195	-3.402	1.00	54.64
ATOM	198	OH	GLY	C	24	60.410	40.339	-2.920	1.00	73.31
ATOM	199	C	PVL	C	25	64.534	35.324	1.332	1.00	17.73
ATOM	200	O	PVL	C	25	65.693	35.692	1.200	1.00	21.35
ATOM	201	CA	PVL	C	25	63.465	36.333	1.535	1.00	26.99
ATOM	202	CB	PVL	C	25	62.040	35.836	1.629	1.00	26.50
ATOM	203	ON	PVL	C	25	63.738	37.533	1.769	1.00	32.90
ATOM	204	N	CYS	C	26	64.218	33.987	1.203	1.00	13.65
ATOM	205	CA	CYS	C	26	65.226	32.982	0.870	1.00	13.69
ATOM	206	CB	CYS	C	26	65.775	32.194	2.112	1.00	19.50
ATOM	207	SG	CYS	C	26	67.153	31.117	1.678	1.00	17.42
ATOM	208	C	CYS	C	26	64.643	32.011	-0.140	1.00	17.14
ATOM	209	O	CYS	C	26	63.688	31.289	0.138	1.00	16.98
ATOM	210	N	ALA	C	27	65.174	32.063	-1.414	1.00	14.97
ATOM	211	CA	ALA	C	27	64.691	31.198	-2.478	1.00	14.51
ATOM	212	C	ALA	C	27	65.506	29.930	-2.416	1.00	11.29
ATOM	213	O	ALA	C	27	66.742	29.944	-2.313	1.00	13.77
ATOM	214	CB	ALA	C	27	64.903	31.930	-3.823	1.00	14.33
ATOM	215	N	ILE	C	28	64.784	28.821	-2.436	1.00	12.96
ATOM	216	CA	ILE	C	28	65.324	27.513	-2.268	1.00	12.54
ATOM	217	C	ILE	C	28	64.763	26.465	-3.281	1.00	13.11
ATOM	218	O	ILE	C	28	63.573	26.396	-3.512	1.00	14.34
ATOM	219	CB	ILE	C	28	64.901	26.977	-0.773	1.00	13.91

ATOM	220	CG1	ILE	C	28	65.435	27.945	0.261	1.00	15.23
ATOM	221	CG2	ILE	C	28	65.386	25.518	-0.497	1.00	16.36
ATOM	222	CD1	ILE	C	28	64.647	27.772	1.637	1.00	17.00
ATOM	223	N	ASP	C	29	65.689	25.727	-3.865	1.00	15.10
ATOM	224	CA	ASP	C	29	65.333	24.657	-4.850	1.00	14.57
ATOM	225	C	ASP	C	29	64.130	23.862	-4.288	1.00	17.57
ATOM	226	O	ASP	C	29	64.177	23.354	-3.130	1.00	15.63
ATOM	227	CB	ASP	C	29	66.532	23.782	-5.032	1.00	14.77
ATOM	228	CG	ASP	C	29	66.330	22.610	-6.002	1.00	14.70
ATOM	229	OD1	ASP	C	29	65.209	22.105	-6.198	1.00	15.75
ATOM	230	OD2	ASP	C	29	67.364	22.123	-6.453	1.00	16.77
ATOM	231	N	GLN	C	30	63.048	23.784	-5.055	1.00	15.71
ATOM	232	CA	GLN	C	30	61.846	23.040	-4.628	1.00	16.19
ATOM	233	C	GLN	C	30	62.169	21.606	-4.152	1.00	17.73
ATOM	234	O	GLN	C	30	61.462	21.048	-3.271	1.00	17.08
ATOM	235	CB	GLN	C	30	60.850	22.897	-5.808	1.00	17.85
ATOM	236	CG	GLN	C	30	59.579	22.183	-5.414	1.00	23.42
ATOM	237	CD	GLN	C	30	58.789	22.951	-4.362	1.00	23.06
ATOM	238	OE1	GLN	C	30	58.361	24.110	-4.575	1.00	21.11
ATOM	239	NE2	GLN	C	30	58.574	22.285	-3.172	1.00	20.59
ATOM	240	N	ASP	C	31	63.168	20.935	-4.730	1.00	16.44
ATOM	241	CA	ASP	C	31	63.520	19.575	-4.314	1.00	16.57
ATOM	242	C	ASP	C	31	63.960	19.625	-2.820	1.00	17.31
ATOM	243	O	ASP	C	31	63.633	18.679	-2.057	1.00	17.32
ATOM	244	CB	ASP	C	31	64.705	18.996	-5.106	1.00	19.02
ATOM	245	CG	ASP	C	31	64.300	18.460	-6.508	1.00	24.47
ATOM	246	OD1	ASP	C	31	63.131	18.037	-6.702	1.00	24.53
ATOM	247	OD2	ASP	C	31	65.223	18.456	-7.380	1.00	22.76
ATOM	248	N	PHE	C	32	64.716	20.662	-2.468	1.00	14.02
ATOM	249	CA	PHE	C	32	65.221	20.820	-1.075	1.00	13.65
ATOM	250	C	PHE	C	32	64.028	21.048	-0.164	1.00	16.12
ATOM	251	O	PHE	C	32	63.971	20.408	0.948	1.00	14.39
ATOM	252	CB	PHE	C	32	66.186	21.980	-0.940	1.00	13.80
ATOM	253	CG	PHE	C	32	67.460	21.862	-1.736	1.00	14.18
ATOM	254	CD1	PHE	C	32	67.825	20.722	-2.462	1.00	15.47
ATOM	255	CD2	PHE	C	32	68.314	22.951	-1.731	1.00	15.29
ATOM	256	CE1	PHE	C	32	69.105	20.705	-3.202	1.00	16.12
ATOM	257	CE2	PHE	C	32	69.515	22.950	-2.452	1.00	16.29
ATOM	258	CZ	PHE	C	32	69.911	21.821	-3.177	1.00	15.53
ATOM	259	N	LEU	C	33	63.106	21.911	-0.561	1.00	15.49
ATOM	260	CA	LEU	C	33	61.887	22.193	0.225	1.00	13.34
ATOM	261	C	LEU	C	33	61.184	20.847	0.455	1.00	17.57
ATOM	262	O	LEU	C	33	60.783	20.497	1.591	1.00	16.65
ATOM	263	CB	LEU	C	33	60.926	23.160	-0.496	1.00	14.40
ATOM	264	CG	LEU	C	33	61.494	24.560	-0.722	1.00	17.89
ATOM	265	CD1	LEU	C	33	60.412	25.420	-1.418	1.00	15.16
ATOM	266	CD2	LEU	C	33	61.823	25.176	0.693	1.00	17.59
ATOM	267	N	ASP	C	34	61.007	20.035	-0.596	1.00	15.41
ATOM	268	CA	ASP	C	34	60.313	18.744	-0.431	1.00	16.06
ATOM	269	C	ASP	C	34	61.016	17.848	0.617	1.00	18.00
ATOM	270	O	ASP	C	34	60.349	17.195	1.433	1.00	18.35
ATOM	271	CB	ASP	C	34	60.390	17.921	-1.770	1.00	18.61
ATOM	272	CG	ASP	C	34	59.489	18.458	-2.875	1.00	24.34
ATOM	273	OD1	ASP	C	34	58.649	19.342	-2.651	1.00	22.17
ATOM	274	OD2	ASP	C	34	59.666	17.915	-4.029	1.00	28.71
ATOM	275	N	ALA	C	35	62.335	17.746	0.547	1.00	13.94
ATOM	276	CA	ALA	C	35	63.094	16.855	1.437	1.00	15.72
ATOM	277	C	ALA	C	35	62.964	17.259	2.887	1.00	17.50
ATOM	278	O	ALA	C	35	62.925	16.383	3.783	1.00	18.53
ATOM	279	CB	ALA	C	35	64.546	16.791	1.044	1.00	16.40

ATOM	280	N	ALA	C	36	62.923	18.572	3.109	1.00	13.80
ATOM	281	CA	ALA	C	36	62.826	19.066	4.512	1.00	14.07
ATOM	282	C	ALA	C	36	61.369	19.265	4.931	1.00	16.21
ATOM	283	O	ALA	C	36	61.109	19.675	6.096	1.00	16.15
ATOM	284	CB	ALA	C	36	63.652	20.361	4.722	1.00	14.23
ATOM	285	N	GLY	C	37	60.408	19.012	4.067	1.00	14.27
ATOM	286	CA	GLY	C	37	59.006	19.193	4.375	1.00	12.78
ATOM	287	C	GLY	C	37	58.621	20.712	4.515	1.00	11.55
ATOM	288	O	GLY	C	37	57.511	21.019	5.022	1.00	13.36
ATOM	289	N	ILE	C	38	59.459	21.637	3.998	1.00	13.57
ATOM	290	CA	ILE	C	38	59.227	23.079	4.058	1.00	13.98
ATOM	291	C	ILE	C	38	58.350	23.496	2.908	1.00	16.32
ATOM	292	O	ILE	C	38	58.538	22.975	1.764	1.00	16.77
ATOM	293	CB	ILE	C	38	60.556	23.845	4.057	1.00	15.34
ATOM	294	CG1	ILE	C	38	61.360	23.434	5.316	1.00	14.55
ATOM	295	CG2	ILE	C	38	60.360	25.362	4.098	1.00	15.27
ATOM	296	CD1	ILE	C	38	62.741	24.006	5.393	1.00	19.63
ATOM	297	N	LEU	C	39	57.410	24.363	3.195	1.00	12.96
ATOM	298	CA	LEU	C	39	56.438	24.870	2.188	1.00	11.40
ATOM	299	C	LEU	C	39	56.789	26.256	1.685	1.00	14.26
ATOM	300	O	LEU	C	39	57.351	27.091	2.351	1.00	13.15
ATOM	301	CB	LEU	C	39	55.018	24.940	2.745	1.00	12.16
ATOM	302	CG	LEU	C	39	54.409	23.724	3.459	1.00	13.32
ATOM	303	CD1	LEU	C	39	53.029	23.936	3.991	1.00	13.99
ATOM	304	CD2	LEU	C	39	54.450	22.512	2.442	1.00	17.01
ATOM	305	N	GLU	C	40	56.438	26.515	0.401	1.00	14.46
ATOM	306	CA	GLU	C	40	56.668	27.856	-0.077	1.00	15.39
ATOM	307	C	GLU	C	40	55.766	28.802	0.813	1.00	13.93
ATOM	308	O	GLU	C	40	54.630	28.488	1.146	1.00	13.92
ATOM	309	CB	GLU	C	40	56.149	27.962	-1.564	1.00	17.33
ATOM	310	CG	GLU	C	40	56.299	29.405	-2.092	1.00	22.86
ATOM	311	CD	GLU	C	40	56.447	29.500	-3.609	1.00	37.57
ATOM	312	OE1	GLU	C	40	55.722	28.731	-4.258	1.00	29.60
ATOM	313	OE2	GLU	C	40	57.284	30.327	-4.101	1.00	24.74
ATOM	314	N	ASN	C	41	56.349	29.944	1.163	1.00	12.53
ATOM	315	CA	ASN	C	41	55.781	31.000	1.960	1.00	12.52
ATOM	316	C	ASN	C	41	55.812	30.629	3.468	1.00	13.84
ATOM	317	O	ASN	C	41	55.228	31.397	4.263	1.00	13.31
ATOM	318	CB	ASN	C	41	54.414	31.386	1.563	1.00	14.21
ATOM	319	CG	ASN	C	41	54.377	31.980	0.096	1.00	18.26
ATOM	320	OD1	ASN	C	41	55.127	32.868	-0.218	1.00	19.96
ATOM	321	ND2	ASN	C	41	53.502	31.428	-0.735	1.00	23.65
ATOM	322	N	GLU	C	42	56.433	29.507	3.815	1.00	12.49
ATOM	323	CA	GLU	C	42	56.487	29.138	5.281	1.00	11.09
ATOM	324	C	GLU	C	42	57.541	29.977	5.920	1.00	12.61
ATOM	325	O	GLU	C	42	58.596	30.268	5.373	1.00	13.32
ATOM	326	CB	GLU	C	42	56.868	27.701	5.408	1.00	11.37
ATOM	327	CG	GLU	C	42	56.806	27.190	6.899	1.00	13.79
ATOM	328	CD	GLU	C	42	57.022	25.698	6.958	1.00	16.86
ATOM	329	OE1	GLU	C	42	57.443	25.053	5.978	1.00	14.48
ATOM	330	OE2	GLU	C	42	56.821	25.073	8.083	1.00	11.57
ATOM	331	N	ALA	C	43	57.338	30.294	7.232	1.00	11.23
ATOM	332	CA	ALA	C	43	58.354	30.979	7.973	1.00	11.52
ATOM	333	C	ALA	C	43	59.543	29.996	8.219	1.00	12.62
ATOM	334	O	ALA	C	43	59.345	28.779	8.496	1.00	11.29
ATOM	335	CB	ALA	C	43	57.767	31.316	9.366	1.00	11.84
ATOM	336	N	ILE	C	44	60.755	30.514	8.084	1.00	10.61
ATOM	337	CA	ILE	C	44	61.976	29.726	8.293	1.00	9.63
ATOM	338	C	ILE	C	44	62.989	30.509	9.135	1.00	11.21
ATOM	339	O	ILE	C	44	63.038	31.761	9.090	1.00	11.77

ATOM	340	CB	ILE	C	44	62.638	29.285	6.929	1.00	11.13
ATOM	341	CG1	ILE	C	44	62.868	30.534	6.052	1.00	12.75
ATOM	342	CG2	ILE	C	44	61.738	28.241	6.300	1.00	11.62
ATOM	343	CD1	ILE	C	44	63.700	30.215	4.745	1.00	16.57
ATOM	344	N	ASP	C	45	63.791	29.766	9.892	1.00	11.18
ATOM	345	CA	ASP	C	45	64.856	30.353	10.646	1.00	10.11
ATOM	346	C	ASP	C	45	66.187	29.921	9.981	1.00	11.65
ATOM	347	O	ASP	C	45	66.334	28.745	9.564	1.00	12.76
ATOM	348	CB	ASP	C	45	64.832	29.780	12.104	1.00	11.49
ATOM	349	CG	ASP	C	45	63.597	30.185	12.832	1.00	12.09
ATOM	350	OD1	ASP	C	45	63.012	31.295	12.643	1.00	13.27
ATOM	351	OD2	ASP	C	45	63.146	29.292	13.666	1.00	16.15
ATOM	352	N	ILE	C	46	67.120	30.860	9.819	1.00	12.45
ATOM	353	CA	ILE	C	46	68.411	30.563	9.169	1.00	11.69
ATOM	354	C	ILE	C	46	69.494	30.864	10.146	1.00	13.15
ATOM	355	O	ILE	C	46	69.566	31.982	10.710	1.00	13.26
ATOM	356	CB	ILE	C	46	68.536	31.422	7.883	1.00	13.14
ATOM	357	CG1	ILE	C	46	67.338	31.096	7.003	1.00	12.28
ATOM	358	CG2	ILE	C	46	69.920	31.132	7.208	1.00	13.37
ATOM	359	CD1	ILE	C	46	67.524	31.730	5.488	1.00	14.34
ATOM	360	N	TRP	C	47	70.322	29.841	10.406	1.00	12.56
ATOM	361	CA	TRP	C	47	71.414	29.944	11.387	1.00	11.59
ATOM	362	C	TRP	C	47	72.717	29.812	10.545	1.00	12.65
ATOM	363	O	TRP	C	47	72.955	28.776	9.937	1.00	13.30
ATOM	364	CB	TRP	C	47	71.265	28.791	12.381	1.00	11.85
ATOM	365	CG	TRP	C	47	69.917	28.832	13.078	1.00	11.21
ATOM	366	CD1	TRP	C	47	69.254	29.942	13.487	1.00	12.57
ATOM	367	CD2	TRP	C	47	69.125	27.705	13.456	1.00	12.14
ATOM	368	NE1	TRP	C	47	68.053	29.581	14.123	1.00	11.88
ATOM	369	CE2	TRP	C	47	67.960	28.215	14.112	1.00	10.79
ATOM	370	CE3	TRP	C	47	69.264	26.331	13.261	1.00	14.11
ATOM	371	CZ2	TRP	C	47	66.930	27.369	14.579	1.00	11.66
ATOM	372	CZ3	TRP	C	47	68.235	25.465	13.766	1.00	14.28
ATOM	373	CH2	TRP	C	47	67.080	26.038	14.410	1.00	14.15
ATOM	374	N	ASN	C	48	73.512	30.856	10.577	1.00	12.67
ATOM	375	CA	ASN	C	48	74.730	30.931	9.784	1.00	14.84
ATOM	376	C	ASN	C	48	75.898	30.311	10.503	1.00	14.53
ATOM	377	O	ASN	C	48	76.456	30.916	11.495	1.00	15.46
ATOM	378	CB	ASN	C	48	74.966	32.379	9.370	1.00	13.17
ATOM	379	CG	ASN	C	48	75.984	32.520	8.231	1.00	12.09
ATOM	380	OD1	ASN	C	48	76.997	31.892	8.252	1.00	14.55
ATOM	381	ND2	ASN	C	48	75.728	33.481	7.353	1.00	14.53
ATOM	382	N	VAL	C	49	76.306	29.138	10.060	1.00	13.24
ATOM	383	CA	VAL	C	49	77.416	28.477	10.667	1.00	13.19
ATOM	384	C	VAL	C	49	78.741	29.222	10.464	1.00	18.14
ATOM	385	O	VAL	C	49	79.658	29.202	11.306	1.00	19.15
ATOM	386	CB	VAL	C	49	77.568	27.013	10.155	1.00	15.64
ATOM	387	CG1	VAL	C	49	78.718	26.315	10.879	1.00	17.34
ATOM	388	CG2	VAL	C	49	76.256	26.221	10.313	1.00	15.21
ATOM	389	N	THR	C	50	78.884	29.888	9.312	1.00	14.80
ATOM	390	CA	THR	C	50	80.115	30.592	9.059	1.00	14.70
ATOM	391	C	THR	C	50	80.332	31.856	9.917	1.00	15.83
ATOM	392	O	THR	C	50	81.434	32.032	10.464	1.00	18.87
ATOM	393	CB	THR	C	50	80.206	30.952	7.521	1.00	18.21
ATOM	394	OG1	THR	C	50	80.146	29.742	6.790	1.00	15.78
ATOM	395	CG2	THR	C	50	81.513	31.639	7.236	1.00	16.82
ATOM	396	N	ASN	C	51	79.334	32.710	10.014	1.00	14.06
ATOM	397	CA	ASN	C	51	79.492	33.962	10.776	1.00	15.31
ATOM	398	C	ASN	C	51	78.715	34.092	12.098	1.00	17.85
ATOM	399	O	ASN	C	51	78.807	35.115	12.755	1.00	17.40

ATOM	400	CB	ASN	C	51	79.229	35.187	9.877	1.00	18.14
ATOM	401	CG	ASN	C	51	77.756	35.329	9.477	1.00	20.44
ATOM	402	OD1	ASN	C	51	76.879	34.705	10.085	1.00	16.68
ATOM	403	ND2	ASN	C	51	77.462	36.172	8.454	1.00	16.78
ATOM	404	N	GLY	C	52	77.954	33.059	12.436	1.00	15.39
ATOM	405	CA	GLY	C	52	77.169	33.081	13.693	1.00	16.35
ATOM	406	C	GLY	C	52	75.868	33.855	13.678	1.00	18.04
ATOM	407	O	GLY	C	52	75.109	33.788	14.680	1.00	15.14
ATOM	408	N	LYS	C	53	75.528	34.597	12.606	1.00	13.62
ATOM	409	CA	LYS	C	53	74.279	35.346	12.571	1.00	13.33
ATOM	410	C	LYS	C	53	73.078	34.419	12.525	1.00	13.70
ATOM	411	O	LYS	C	53	73.156	33.312	11.988	1.00	13.57
ATOM	412	CB	LYS	C	53	74.226	36.376	11.407	1.00	15.27
ATOM	413	CG	LYS	C	53	75.408	37.304	11.460	1.00	16.18
ATOM	414	CD	LYS	C	53	75.235	38.411	10.445	1.00	18.83
ATOM	415	CE	LYS	C	53	76.538	39.222	10.332	1.00	24.88
ATOM	416	NZ	LYS	C	53	76.488	40.240	9.151	1.00	24.28
ATOM	417	N	ARG	C	54	71.957	34.851	13.130	1.00	12.69
ATOM	418	CA	ARG	C	54	70.720	34.077	13.202	1.00	11.88
ATOM	419	C	ARG	C	54	69.563	35.017	12.837	1.00	14.37
ATOM	420	O	ARG	C	54	69.422	36.109	13.368	1.00	13.79
ATOM	421	CB	ARG	C	54	70.513	33.544	14.658	1.00	11.58
ATOM	422	CG	ARG	C	54	71.674	32.735	15.081	1.00	12.91
ATOM	423	CD	ARG	C	54	71.473	32.182	16.577	1.00	13.98
ATOM	424	NE	ARG	C	54	70.621	31.016	16.648	1.00	15.65
ATOM	425	CZ	ARG	C	54	71.030	29.772	16.432	1.00	13.20
ATOM	426	NH1	ARG	C	54	72.320	29.537	16.081	1.00	13.97
ATOM	427	NH2	ARG	C	54	70.206	28.733	16.554	1.00	12.47
ATOM	428	N	PHE	C	55	68.708	34.614	11.897	1.00	13.21
ATOM	429	CA	PHE	C	55	67.605	35.481	11.482	1.00	11.72
ATOM	430	C	PHE	C	55	66.418	34.634	11.006	1.00	12.09
ATOM	431	O	PHE	C	55	66.591	33.396	10.737	1.00	14.53
ATOM	432	CB	PHE	C	55	68.046	36.473	10.368	1.00	12.81
ATOM	433	CG	PHE	C	55	68.562	35.804	9.087	1.00	14.26
ATOM	434	CD1	PHE	C	55	69.846	35.318	9.008	1.00	15.91
ATOM	435	CD2	PHE	C	55	67.757	35.761	7.976	1.00	16.89
ATOM	436	CE1	PHE	C	55	70.335	34.741	7.814	1.00	18.73
ATOM	437	CE2	PHE	C	55	68.244	35.194	6.797	1.00	18.14
ATOM	438	CZ	PHE	C	55	69.487	34.707	6.724	1.00	16.81
ATOM	439	N	SER	C	56	65.271	35.285	10.899	1.00	12.30
ATOM	440	CA	SER	C	56	64.027	34.624	10.507	1.00	11.60
ATOM	441	C	SER	C	56	63.434	35.336	9.280	1.00	13.08
ATOM	442	O	SER	C	56	63.432	36.539	9.216	1.00	12.92
ATOM	443	CB	SER	C	56	63.017	34.612	11.646	1.00	14.04
ATOM	444	OG	SER	C	56	63.603	33.905	12.760	1.00	17.74
ATOM	445	N	THR	C	57	62.982	34.543	8.325	1.00	12.51
ATOM	446	CA	THR	C	57	62.408	35.094	7.083	1.00	15.14
ATOM	447	C	THR	C	57	61.340	34.103	6.578	1.00	16.57
ATOM	448	O	THR	C	57	60.653	33.469	7.397	1.00	13.36
ATOM	449	CB	THR	C	57	63.513	35.345	6.067	1.00	17.35
ATOM	450	OG1	THR	C	57	62.937	36.006	4.924	1.00	17.51
ATOM	451	CG2	THR	C	57	64.314	34.105	5.666	1.00	19.79
ATOM	452	N	TYR	C	58	61.118	33.960	5.247	1.00	13.07
ATOM	453	CA	TYR	C	58	60.120	33.001	4.744	1.00	11.86
ATOM	454	C	TYR	C	58	60.721	32.381	3.453	1.00	14.46
ATOM	455	O	TYR	C	58	61.629	32.949	2.879	1.00	14.80
ATOM	456	CB	TYR	C	58	58.762	33.591	4.472	1.00	11.64
ATOM	457	CG	TYR	C	58	58.754	34.679	3.414	1.00	14.08
ATOM	458	CD1	TYR	C	58	59.116	35.983	3.729	1.00	14.47
ATOM	459	CD2	TYR	C	58	58.407	34.360	2.083	1.00	16.79

ATOM	460	CE1	TYR	C	58	59.123	36.982	2.767	1.00	19.79
ATOM	461	CE2	TYR	C	58	58.408	35.385	1.101	1.00	15.79
ATOM	462	CZ	TYR	C	58	58.772	36.658	1.465	1.00	22.24
ATOM	463	OH	TYR	C	58	58.773	37.582	0.406	1.00	23.11
ATOM	464	N	ALA	C	59	60.236	31.199	3.113	1.00	11.72
ATOM	465	CA	ALA	C	59	60.747	30.471	1.952	1.00	12.72
ATOM	466	C	ALA	C	59	60.040	30.828	0.681	1.00	12.49
ATOM	467	O	ALA	C	59	58.820	30.922	0.629	1.00	13.37
ATOM	468	CB	ALA	C	59	60.532	28.933	2.179	1.00	13.81
ATOM	469	N	ILE	C	60	60.887	30.962	-0.360	1.00	15.14
ATOM	470	CA	ILE	C	60	60.387	31.207	-1.760	1.00	16.33
ATOM	471	C	ILE	C	60	60.878	29.978	-2.563	1.00	16.77
ATOM	472	O	ILE	C	60	62.007	29.525	-2.396	1.00	14.68
ATOM	473	CB	ILE	C	60	61.069	32.427	-2.340	1.00	18.30
ATOM	474	CG1	ILE	C	60	60.607	33.708	-1.635	1.00	19.09
ATOM	475	CG2	ILE	C	60	60.811	32.500	-3.911	1.00	21.06
ATOM	476	CD1	ILE	C	60	61.497	34.913	-1.895	1.00	26.31
ATOM	477	N	ALA	C	61	60.014	29.412	-3.422	1.00	15.66
ATOM	478	CA	ALA	C	61	60.493	28.249	-4.180	1.00	15.73
ATOM	479	C	ALA	C	61	61.328	28.696	-5.413	1.00	18.47
ATOM	480	O	ALA	C	61	60.970	29.648	-6.096	1.00	23.19
ATOM	481	CB	ALA	C	61	59.337	27.383	-4.642	1.00	17.99
ATOM	482	N	ALA	C	62	62.430	28.006	-5.607	1.00	14.95
ATOM	483	CA	ALA	C	62	63.342	28.198	-6.774	1.00	14.55
ATOM	484	C	ALA	C	62	63.068	26.946	-7.605	1.00	18.92
ATOM	485	O	ALA	C	62	62.551	25.909	-7.178	1.00	17.86
ATOM	486	CB	ALA	C	62	64.817	28.259	-6.403	1.00	13.98
ATOM	487	N	GLU	C	63	63.424	27.072	-8.904	1.00	17.78
ATOM	488	CA	GLU	C	63	63.220	25.977	-9.834	1.00	19.52
ATOM	489	C	GLU	C	63	63.779	24.635	-9.365	1.00	19.81
ATOM	490	O	GLU	C	63	64.894	24.571	-8.868	1.00	17.13
ATOM	491	CB	GLU	C	63	63.968	26.354	-11.140	1.00	21.37
ATOM	492	CG	GLU	C	63	63.779	25.342	-12.296	1.00	29.86
ATOM	493	CD	GLU	C	63	64.980	25.283	-13.255	1.00	53.22
ATOM	494	OE1	GLU	C	63	65.920	26.108	-13.149	1.00	44.04
ATOM	495	OE2	GLU	C	63	64.964	24.394	-14.129	1.00	43.79
ATOM	496	N	ARG	C	64	63.012	23.575	-9.561	1.00	16.26
ATOM	497	CA	ARG	C	64	63.425	22.245	-9.201	1.00	16.34
ATOM	498	C	ARG	C	64	64.723	21.863	-9.911	1.00	21.13
ATOM	499	O	ARG	C	64	64.809	21.970	-11.168	1.00	20.36
ATOM	500	CB	ARG	C	64	62.326	21.232	-9.503	1.00	19.26
ATOM	501	CG	ARG	C	64	62.635	19.890	-8.963	1.00	26.38
ATOM	502	CD	ARG	C	64	61.521	18.875	-9.196	1.00	27.64
ATOM	503	NE	ARG	C	64	60.171	19.286	-8.819	1.00	26.53
ATOM	504	CZ	ARG	C	64	59.662	19.154	-7.585	1.00	41.54
ATOM	505	NH1	ARG	C	64	60.408	18.669	-6.578	1.00	23.51
ATOM	506	NH2	ARG	C	64	58.421	19.526	-7.351	1.00	30.75
ATOM	507	N	GLY	C	65	65.728	21.436	-9.177	1.00	17.09
ATOM	508	CA	GLY	C	65	67.000	21.022	-9.721	1.00	17.60
ATOM	509	C	GLY	C	65	68.038	22.140	-9.853	1.00	18.83
ATOM	510	O	GLY	C	65	69.192	21.885	-10.218	1.00	20.21
ATOM	511	N	SER	C	66	67.650	23.380	-9.543	1.00	16.18
ATOM	512	CA	SER	C	66	68.539	24.515	-9.627	1.00	15.57
ATOM	513	C	SER	C	66	69.606	24.577	-8.516	1.00	19.13
ATOM	514	O	SER	C	66	70.673	25.179	-8.654	1.00	18.34
ATOM	515	CB	SER	C	66	67.764	25.795	-9.596	1.00	18.61
ATOM	516	OG	SER	C	66	67.136	26.006	-8.280	1.00	17.83
ATOM	517	N	ARG	C	67	69.272	23.904	-7.390	1.00	16.53
ATOM	518	CA	ARG	C	67	70.164	23.877	-6.187	1.00	17.76
ATOM	519	C	ARG	C	67	70.423	25.285	-5.633	1.00	14.93

ATOM	520	O	ARG	C	67	71.423	25.507	-4.998	1.00	16.56
ATOM	521	CB	ARG	C	67	71.476	23.153	-6.456	1.00	15.58
ATOM	522	CG	ARG	C	67	71.298	21.685	-6.865	1.00	14.91
ATOM	523	CD	ARG	C	67	72.533	20.909	-6.767	1.00	13.81
ATOM	524	NE	ARG	C	67	72.322	19.522	-7.249	1.00	16.78
ATOM	525	CZ	ARG	C	67	73.219	18.551	-7.123	1.00	18.26
ATOM	526	NH1	ARG	C	67	74.395	18.751	-6.546	1.00	18.16
ATOM	527	NH2	ARG	C	67	72.944	17.336	-7.609	1.00	19.31
ATOM	528	N	ILE	C	68	69.503	26.201	-5.884	1.00	13.92
ATOM	529	CA	ILE	C	68	69.659	27.584	-5.447	1.00	13.11
ATOM	530	C	ILE	C	68	69.325	27.709	-3.918	1.00	14.96
ATOM	531	O	ILE	C	68	68.385	27.063	-3.430	1.00	16.08
ATOM	532	CB	ILE	C	68	68.680	28.483	-6.228	1.00	16.07
ATOM	533	CG1	ILE	C	68	69.177	28.633	-7.743	1.00	15.43
ATOM	534	CG2	ILE	C	68	68.517	29.887	-5.539	1.00	14.91
ATOM	535	CD1	ILE	C	68	68.162	29.265	-8.585	1.00	17.12
ATOM	536	N	ILE	C	69	70.116	28.547	-3.278	1.00	15.79
ATOM	537	CA	ILE	C	69	69.921	29.021	-1.887	1.00	14.43
ATOM	538	C	ILE	C	69	70.273	30.521	-2.099	1.00	12.91
ATOM	539	O	ILE	C	69	71.469	30.897	-2.053	1.00	16.10
ATOM	540	CB	ILE	C	69	70.826	28.392	-0.867	1.00	14.38
ATOM	541	CG1	ILE	C	69	70.632	26.859	-0.742	1.00	14.18
ATOM	542	CG2	ILE	C	69	70.524	29.042	0.545	1.00	14.77
ATOM	543	CD1	ILE	C	69	69.240	26.399	-0.207	1.00	13.25
ATOM	544	N	SER	C	70	69.266	31.361	-2.315	1.00	12.61
ATOM	545	CA	SER	C	70	69.474	32.776	-2.545	1.00	12.79
ATOM	546	C	SER	C	70	68.897	33.612	-1.365	1.00	16.65
ATOM	547	O	SER	C	70	67.703	33.574	-1.101	1.00	16.44
ATOM	548	CB	SER	C	70	68.786	33.187	-3.877	1.00	17.19
ATOM	549	OG	SER	C	70	69.055	34.583	-4.178	1.00	19.28
ATOM	550	N	VAL	C	71	69.763	34.375	-0.735	1.00	16.77
ATOM	551	CA	VAL	C	71	69.353	35.237	0.411	1.00	16.54
ATOM	552	C	VAL	C	71	69.046	36.611	-0.216	1.00	18.47
ATOM	553	O	VAL	C	71	69.938	37.276	-0.785	1.00	20.32
ATOM	554	CB	VAL	C	71	70.489	35.218	1.485	1.00	21.34
ATOM	555	CG1	VAL	C	71	70.168	36.151	2.628	1.00	23.85
ATOM	556	CG2	VAL	C	71	70.661	33.816	2.075	1.00	21.90
ATOM	557	N	ASN	C	72	67.793	37.013	-0.156	1.00	17.21
ATOM	558	CA	ASN	C	72	67.310	38.229	-0.774	1.00	18.06
ATOM	559	C	ASN	C	72	66.822	39.292	0.185	1.00	22.03
ATOM	560	O	ASN	C	72	66.550	38.985	1.364	1.00	20.77
ATOM	561	CB	ASN	C	72	66.111	37.862	-1.684	1.00	15.71
ATOM	562	CG	ASN	C	72	66.479	36.805	-2.771	1.00	21.14
ATOM	563	OD1	ASN	C	72	67.625	36.673	-3.142	1.00	22.76
ATOM	564	ND2	ASN	C	72	65.471	36.043	-3.192	1.00	26.84
ATOM	565	N	GLY	C	73	66.680	40.519	-0.296	1.00	17.96
ATOM	566	CA	GLY	C	73	66.191	41.609	0.547	1.00	17.13
ATOM	567	C	GLY	C	73	67.152	41.925	1.662	1.00	17.10
ATOM	568	O	GLY	C	73	68.358	41.772	1.548	1.00	17.56
ATOM	569	N	ALA	C	74	66.585	42.379	2.783	1.00	16.81
ATOM	570	CA	ALA	C	74	67.448	42.743	3.926	1.00	16.63
ATOM	571	C	ALA	C	74	68.307	41.588	4.409	1.00	17.98
ATOM	572	O	ALA	C	74	69.403	41.809	4.948	1.00	17.87
ATOM	573	CB	ALA	C	74	66.585	43.261	5.083	1.00	16.76
ATOM	574	N	ALA	C	75	67.829	40.348	4.210	1.00	16.77
ATOM	575	CA	ALA	C	75	68.603	39.156	4.626	1.00	17.69
ATOM	576	C	ALA	C	75	70.019	39.079	3.999	1.00	17.68
ATOM	577	O	ALA	C	75	70.898	38.411	4.507	1.00	16.79
ATOM	578	CB	ALA	C	75	67.861	37.907	4.282	1.00	20.55
ATOM	579	N	ALA	C	76	70.216	39.775	2.856	1.00	16.67

ATOM	580	CA	ALA	C	76	71.535	39.737	2.230	1.00	17.52
ATOM	581	C	ALA	C	76	72.644	40.382	3.121	1.00	17.22
ATOM	582	O	ALA	C	76	73.840	40.202	2.886	1.00	18.09
ATOM	583	CB	ALA	C	76	71.482	40.359	0.797	1.00	18.29
ATOM	584	N	HIS	C	77	72.232	41.101	4.193	1.00	15.19
ATOM	585	CA	HIS	C	77	73.203	41.686	5.120	1.00	16.72
ATOM	586	C	HIS	C	77	73.627	40.623	6.163	1.00	16.17
ATOM	587	O	HIS	C	77	74.587	40.860	6.914	1.00	18.25
ATOM	588	CB	HIS	C	77	72.502	42.778	5.963	1.00	18.31
ATOM	589	CG	HIS	C	77	72.336	44.077	5.261	1.00	21.21
ATOM	590	ND1	HIS	C	77	73.368	44.963	5.118	1.00	25.21
ATOM	591	CD2	HIS	C	77	71.258	44.654	4.687	1.00	22.31
ATOM	592	CE1	HIS	C	77	72.940	46.030	4.463	1.00	23.74
ATOM	593	NE2	HIS	C	77	71.663	45.876	4.200	1.00	22.33
ATOM	594	N	CYS	C	78	72.921	39.495	6.201	1.00	14.86
ATOM	595	CA	CYS	C	78	73.192	38.449	7.199	1.00	16.42
ATOM	596	C	CYS	C	78	73.868	37.192	6.701	1.00	16.96
ATOM	597	O	CYS	C	78	74.290	36.294	7.516	1.00	16.97
ATOM	598	CB	CYS	C	78	71.873	38.018	7.877	1.00	16.76
ATOM	599	SG	CYS	C	78	70.910	39.411	8.622	1.00	22.74
ATOM	600	N	ALA	C	79	73.983	37.044	5.346	1.00	14.78
ATOM	601	CA	ALA	C	79	74.626	35.854	4.795	1.00	14.85
ATOM	602	C	ALA	C	79	75.204	36.282	3.435	1.00	15.30
ATOM	603	O	ALA	C	79	74.676	37.213	2.822	1.00	16.51
ATOM	604	CB	ALA	C	79	73.652	34.707	4.608	1.00	15.77
ATOM	605	N	SER	C	80	76.281	35.597	3.082	1.00	13.90
ATOM	606	CA	SER	C	80	77.009	35.855	1.804	1.00	13.46
ATOM	607	C	SER	C	80	77.182	34.588	1.039	1.00	17.54
ATOM	608	O	SER	C	80	77.156	33.497	1.573	1.00	16.85
ATOM	609	CB	SER	C	80	78.368	36.434	2.130	1.00	17.79
ATOM	610	OG	SER	C	80	78.214	37.661	2.852	1.00	18.84
ATOM	611	N	VAL	C	81	77.403	34.738	-0.290	1.00	15.99
ATOM	612	CA	VAL	C	81	77.636	33.575	-1.121	1.00	14.74
ATOM	613	C	VAL	C	81	78.865	32.845	-0.571	1.00	14.78
ATOM	614	O	VAL	C	81	79.915	33.417	-0.317	1.00	15.81
ATOM	615	CB	VAL	C	81	77.941	34.058	-2.623	1.00	14.01
ATOM	616	CG1	VAL	C	81	78.354	32.825	-3.456	1.00	15.95
ATOM	617	CG2	VAL	C	81	76.706	34.650	-3.234	1.00	15.67
ATOM	618	N	GLY	C	82	78.740	31.543	-0.346	1.00	14.65
ATOM	619	CA	GLY	C	82	79.809	30.766	0.200	1.00	14.30
ATOM	620	C	GLY	C	82	79.558	30.358	1.673	1.00	16.91
ATOM	621	O	GLY	C	82	80.116	29.368	2.122	1.00	15.50
ATOM	622	N	ASP	C	83	78.746	31.145	2.355	1.00	14.93
ATOM	623	CA	ASP	C	83	78.465	30.803	3.792	1.00	13.74
ATOM	624	C	ASP	C	83	77.699	29.490	3.879	1.00	14.63
ATOM	625	O	ASP	C	83	76.858	29.163	3.011	1.00	15.91
ATOM	626	CB	ASP	C	83	77.586	31.900	4.467	1.00	13.28
ATOM	627	CG	ASP	C	83	78.339	33.192	4.782	1.00	12.11
ATOM	628	OD1	ASP	C	83	79.600	33.269	4.679	1.00	15.32
ATOM	629	OD2	ASP	C	83	77.591	34.161	5.119	1.00	15.76
ATOM	630	N	ILE	C	84	77.970	28.743	4.968	1.00	14.29
ATOM	631	CA	ILE	C	84	77.296	27.473	5.239	1.00	13.65
ATOM	632	C	ILE	C	84	76.184	27.799	6.282	1.00	13.60
ATOM	633	O	ILE	C	84	76.469	28.474	7.272	1.00	15.62
ATOM	634	CB	ILE	C	84	78.287	26.496	5.913	1.00	16.83
ATOM	635	CG1	ILE	C	84	79.463	26.115	4.939	1.00	17.52
ATOM	636	CG2	ILE	C	84	77.560	25.231	6.346	1.00	19.25
ATOM	637	CD1	ILE	C	84	78.981	25.389	3.679	1.00	21.07
ATOM	638	N	VAL	C	85	74.976	27.392	6.001	1.00	12.41
ATOM	639	CA	VAL	C	85	73.864	27.713	6.910	1.00	12.94

ATOM	640	C	VAL	C	85	72.991	26.532	7.153	1.00	15.89
ATOM	641	O	VAL	C	85	73.039	25.474	6.469	1.00	14.01
ATOM	642	CB	VAL	C	85	72.979	28.838	6.312	1.00	14.37
ATOM	643	CG1	VAL	C	85	73.801	30.088	5.901	1.00	13.95
ATOM	644	CG2	VAL	C	85	72.180	28.356	5.045	1.00	14.77
ATOM	645	N	ILE	C	86	72.116	26.676	8.178	1.00	13.28
ATOM	646	CA	ILE	C	86	71.158	25.631	8.523	1.00	13.39
ATOM	647	C	ILE	C	86	69.809	26.347	8.420	1.00	14.02
ATOM	648	O	ILE	C	86	69.643	27.439	8.961	1.00	13.98
ATOM	649	CB	ILE	C	86	71.391	25.081	9.985	1.00	13.99
ATOM	650	CG1	ILE	C	86	72.703	24.242	10.022	1.00	17.59
ATOM	651	CG2	ILE	C	86	70.181	24.220	10.367	1.00	15.22
ATOM	652	CD1	ILE	C	86	73.325	24.108	11.423	1.00	22.03
ATOM	653	N	ILE	C	87	68.861	25.804	7.637	1.00	12.05
ATOM	654	CA	ILE	C	87	67.560	26.410	7.449	1.00	11.27
ATOM	655	C	ILE	C	87	66.521	25.488	8.056	1.00	12.08
ATOM	656	O	ILE	C	87	66.411	24.300	7.711	1.00	13.19
ATOM	657	CB	ILE	C	87	67.259	26.629	5.881	1.00	12.91
ATOM	658	CG1	ILE	C	87	68.381	27.458	5.331	1.00	14.33
ATOM	659	CG2	ILE	C	87	65.903	27.272	5.724	1.00	14.68
ATOM	660	CD1	ILE	C	87	68.240	27.670	3.726	1.00	14.91
ATOM	661	N	ALA	C	88	65.718	26.045	9.004	1.00	11.17
ATOM	662	CA	ALA	C	88	64.724	25.224	9.662	1.00	11.51
ATOM	663	C	ALA	C	88	63.339	25.757	9.674	1.00	11.06
ATOM	664	O	ALA	C	88	63.146	26.990	9.596	1.00	12.85
ATOM	665	CB	ALA	C	88	65.208	25.134	11.204	1.00	12.18
ATOM	666	N	SER	C	89	62.321	24.892	9.833	1.00	11.32
ATOM	667	CA	SER	C	89	60.945	25.386	10.017	1.00	11.17
ATOM	668	C	SER	C	89	60.407	24.644	11.248	1.00	11.44
ATOM	669	O	SER	C	89	60.891	23.539	11.573	1.00	11.04
ATOM	670	CB	SER	C	89	59.986	25.246	8.807	1.00	14.68
ATOM	671	OG	SER	C	89	59.409	23.939	8.749	1.00	13.56
ATOM	672	N	PHE	C	90	59.489	25.340	11.926	1.00	11.58
ATOM	673	CA	PHE	C	90	58.878	24.772	13.154	1.00	10.03
ATOM	674	C	PHE	C	90	57.391	24.743	13.006	1.00	11.41
ATOM	675	O	PHE	C	90	56.780	25.662	12.350	1.00	12.95
ATOM	676	CB	PHE	C	90	59.257	25.677	14.348	1.00	10.86
ATOM	677	CG	PHE	C	90	60.681	25.536	14.776	1.00	11.25
ATOM	678	CD1	PHE	C	90	61.724	26.266	14.169	1.00	12.54
ATOM	679	CD2	PHE	C	90	61.016	24.612	15.810	1.00	13.88
ATOM	680	CE1	PHE	C	90	63.094	26.079	14.613	1.00	12.35
ATOM	681	CE2	PHE	C	90	62.289	24.431	16.247	1.00	13.61
ATOM	682	CZ	PHE	C	90	63.373	25.138	15.672	1.00	12.98
ATOM	683	N	VAL	C	91	56.768	23.720	13.608	1.00	9.83
ATOM	684	CA	VAL	C	91	55.315	23.572	13.573	1.00	10.22
ATOM	685	C	VAL	C	91	54.795	23.312	14.993	1.00	14.03
ATOM	686	O	VAL	C	91	55.606	22.962	15.893	1.00	13.50
ATOM	687	CB	VAL	C	91	54.804	22.401	12.688	1.00	13.62
ATOM	688	CG1	VAL	C	91	55.015	22.757	11.190	1.00	15.08
ATOM	689	CG2	VAL	C	91	55.481	21.082	13.064	1.00	13.05
ATOM	690	N	THR	C	92	53.528	23.542	15.175	1.00	12.76
ATOM	691	CA	THR	C	92	52.916	23.289	16.511	1.00	11.56
ATOM	692	C	THR	C	92	51.985	22.099	16.437	1.00	13.31
ATOM	693	O	THR	C	92	51.347	21.772	15.395	1.00	13.08
ATOM	694	CB	THR	C	92	52.237	24.503	17.160	1.00	12.64
ATOM	695	OG1	THR	C	92	51.102	24.918	16.359	1.00	16.06
ATOM	696	CG2	THR	C	92	53.186	25.697	17.314	1.00	13.80
ATOM	697	N	MET	C	93	51.881	21.327	17.562	1.00	11.69
ATOM	698	CA	MET	C	93	51.013	20.142	17.639	1.00	11.35
ATOM	699	C	MET	C	93	50.872	19.828	19.145	1.00	14.45

ATOM	700	O	MET	C	93	51.654	20.324	19.951	1.00	13.44
ATOM	701	CB	MET	C	93	51.697	18.907	16.955	1.00	12.85
ATOM	702	CG	MET	C	93	53.062	18.586	17.608	1.00	13.91
ATOM	703	SD	MET	C	93	54.059	17.382	16.687	1.00	14.46
ATOM	704	CE	MET	C	93	54.523	18.473	15.286	1.00	14.10
ATOM	705	N	PRO	C	94	49.873	19.055	19.455	1.00	12.36
ATOM	706	CA	PRO	C	94	49.648	18.670	20.865	1.00	12.35
ATOM	707	C	PRO	C	94	50.877	17.883	21.402	1.00	15.66
ATOM	708	O	PRO	C	94	51.630	17.195	20.717	1.00	14.35
ATOM	709	CB	PRO	C	94	48.504	17.712	20.781	1.00	13.86
ATOM	710	CG	PRO	C	94	47.676	18.206	19.582	1.00	15.72
ATOM	711	CD	PRO	C	94	48.832	18.461	18.595	1.00	12.82
ATOM	712	N	ASP	C	95	51.023	17.929	22.751	1.00	14.03
ATOM	713	CA	ASP	C	95	52.125	17.208	23.352	1.00	15.39
ATOM	714	C	ASP	C	95	52.288	15.721	22.997	1.00	16.06
ATOM	715	O	ASP	C	95	53.415	15.216	22.827	1.00	16.29
ATOM	716	CB	ASP	C	95	51.982	17.327	24.883	1.00	15.44
ATOM	717	CG	ASP	C	95	53.209	16.791	25.618	1.00	15.85
ATOM	718	OD1	ASP	C	95	54.314	17.367	25.497	1.00	14.33
ATOM	719	OD2	ASP	C	95	53.073	15.750	26.345	1.00	18.70
ATOM	720	N	GLU	C	96	51.181	14.987	22.922	1.00	15.70
ATOM	721	CA	GLU	C	96	51.283	13.563	22.604	1.00	14.32
ATOM	722	C	GLU	C	96	51.905	13.295	21.236	1.00	18.35
ATOM	723	O	GLU	C	96	52.794	12.468	21.100	1.00	17.78
ATOM	724	CB	GLU	C	96	49.944	12.850	22.791	1.00	16.31
ATOM	725	CG	GLU	C	96	50.012	11.377	22.421	1.00	22.63
ATOM	726	CD	GLU	C	96	48.701	10.594	22.718	1.00	23.98
ATOM	727	OE1	GLU	C	96	47.699	11.210	23.080	1.00	25.84
ATOM	728	OE2	GLU	C	96	48.703	9.363	22.540	1.00	30.53
ATOM	729	N	GLU	C	97	51.419	14.032	20.241	1.00	15.16
ATOM	730	CA	GLU	C	97	52.004	13.852	18.911	1.00	15.52
ATOM	731	C	GLU	C	97	53.491	14.296	18.936	1.00	13.99
ATOM	732	O	GLU	C	97	54.332	13.695	18.293	1.00	16.67
ATOM	733	CB	GLU	C	97	51.202	14.706	17.929	1.00	15.35
ATOM	734	CG	GLU	C	97	51.780	14.636	16.496	1.00	17.59
ATOM	735	CD	GLU	C	97	50.924	15.416	15.525	1.00	22.36
ATOM	736	OE1	GLU	C	97	49.940	16.082	15.936	1.00	17.71
ATOM	737	OE2	GLU	C	97	51.268	15.305	14.305	1.00	22.62
ATOM	738	N	ALA	C	98	53.816	15.379	19.663	1.00	13.03
ATOM	739	CA	ALA	C	98	55.185	15.883	19.750	1.00	12.71
ATOM	740	C	ALA	C	98	56.174	14.859	20.323	1.00	15.63
ATOM	741	O	ALA	C	98	57.339	14.809	19.952	1.00	14.36
ATOM	742	CB	ALA	C	98	55.199	17.161	20.596	1.00	14.85
ATOM	743	N	ARG	C	99	55.689	13.987	21.252	1.00	14.05
ATOM	744	CA	ARG	C	99	56.579	13.018	21.842	1.00	15.96
ATOM	745	C	ARG	C	99	57.090	11.936	20.924	1.00	17.44
ATOM	746	O	ARG	C	99	58.103	11.307	21.251	1.00	21.21
ATOM	747	CB	ARG	C	99	55.968	12.422	23.153	1.00	17.37
ATOM	748	CG	ARG	C	99	55.949	13.457	24.271	1.00	16.32
ATOM	749	CD	ARG	C	99	55.383	12.905	25.632	1.00	16.45
ATOM	750	NE	ARG	C	99	53.933	12.912	25.712	1.00	14.75
ATOM	751	CZ	ARG	C	99	53.157	11.860	25.584	1.00	13.61
ATOM	752	NH1	ARG	C	99	53.688	10.668	25.371	1.00	16.09
ATOM	753	NH2	ARG	C	99	51.846	11.988	25.703	1.00	18.40
ATOM	754	N	THR	C	100	56.438	11.713	19.788	1.00	16.42
ATOM	755	CA	THR	C	100	56.970	10.700	18.869	1.00	16.33
ATOM	756	C	THR	C	100	57.108	11.310	17.469	1.00	19.97
ATOM	757	O	THR	C	100	57.162	10.569	16.457	1.00	20.03
ATOM	758	CB	THR	C	100	56.147	9.435	18.772	1.00	21.91
ATOM	759	OG1	THR	C	100	54.764	9.744	18.520	1.00	20.66

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ATOM    760  CG2 THR C 100      56.224   8.675  20.128  1.00 22.68
ATOM    761  N   TRP C 101      57.180  12.634  17.437  1.00 17.87
ATOM    762  CA  TRP C 101      57.321  13.322  16.115  1.00 16.71
ATOM    763  C   TRP C 101      58.708  13.111  15.528  1.00 19.04
ATOM    764  O   TRP C 101      59.710  13.152  16.246  1.00 17.05
ATOM    765  CB  TRP C 101      57.100  14.825  16.331  1.00 14.65
ATOM    766  CG  TRP C 101      57.469  15.675  15.092  1.00 14.16
ATOM    767  CD1 TRP C 101      58.521  16.473  14.986  1.00 16.31
ATOM    768  CD2 TRP C 101      56.693  15.803  13.887  1.00 16.31
ATOM    769  NE1 TRP C 101      58.514  17.103  13.701  1.00 15.49
ATOM    770  CE2 TRP C 101      57.398  16.686  13.043  1.00 17.23
ATOM    771  CE3 TRP C 101      55.500  15.234  13.424  1.00 19.60
ATOM    772  CZ2 TRP C 101      56.935  17.023  11.749  1.00 18.02
ATOM    773  CZ3 TRP C 101      55.020  15.590  12.147  1.00 21.23
ATOM    774  CH2 TRP C 101      55.747  16.467  11.343  1.00 21.41
ATOM    775  N   ARG C 102      58.788  12.895  14.174  1.00 15.76
ATOM    776  CA  ARG C 102      60.114  12.715  13.551  1.00 16.64
ATOM    777  C   ARG C 102      60.358  13.856  12.511  1.00 14.79
ATOM    778  O   ARG C 102      59.671  13.858  11.470  1.00 17.03
ATOM    779  CB  ARG C 102      60.181  11.375  12.823  1.00 17.42
ATOM    780  CG  ARG C 102      59.934  10.169  13.728  1.00 24.67
ATOM    781  CD  ARG C 102      60.918  10.190  14.864  1.00 40.94
ATOM    782  NE  ARG C 102      60.647   9.111  15.815  1.00 58.76
ATOM    783  CZ  ARG C 102      60.403   9.287  17.118  1.00 65.94
ATOM    784  NH1 ARG C 102      60.393  10.518  17.651  1.00 46.00
ATOM    785  NH2 ARG C 102      60.162   8.231  17.890  1.00 52.57
ATOM    786  N   PRO C 103      61.262  14.768  12.787  1.00 15.12
ATOM    787  CA  PRO C 103      61.499  15.893  11.838  1.00 13.53
ATOM    788  C   PRO C 103      62.051  15.360  10.512  1.00 15.29
ATOM    789  O   PRO C 103      62.678  14.328  10.477  1.00 16.02
ATOM    790  CB  PRO C 103      62.536  16.744  12.516  1.00 14.34
ATOM    791  CG  PRO C 103      62.357  16.404  14.069  1.00 18.46
ATOM    792  CD  PRO C 103      62.024  14.929  14.038  1.00 15.59
ATOM    793  N   ASN C 104      61.797  16.147   9.439  1.00 14.28
ATOM    794  CA  ASN C 104      62.283  15.811   8.088  1.00 13.04
ATOM    795  C   ASN C 104      63.643  16.508   7.924  1.00 14.43
ATOM    796  O   ASN C 104      63.701  17.742   7.661  1.00 13.98
ATOM    797  CB  ASN C 104      61.242  16.325   7.131  1.00 12.98
ATOM    798  CG  ASN C 104      59.954  15.602   7.276  1.00 15.09
ATOM    799  OD1 ASN C 104      59.914  14.364   7.131  1.00 17.92
ATOM    800  ND2 ASN C 104      58.886  16.310   7.628  1.00 16.93
ATOM    801  N   VAL C 105      64.733  15.763   8.113  1.00 14.40
ATOM    802  CA  VAL C 105      66.051  16.308   8.052  1.00 15.19
ATOM    803  C   VAL C 105      66.791  15.897   6.794  1.00 18.79
ATOM    804  O   VAL C 105      66.870  14.705   6.477  1.00 20.46
ATOM    805  CB  VAL C 105      66.898  15.862   9.252  1.00 18.28
ATOM    806  CG1 VAL C 105      68.294  16.482   9.195  1.00 20.67
ATOM    807  CG2 VAL C 105      66.189  16.312  10.600  1.00 17.51
ATOM    808  N   ALA C 106      67.321  16.899   6.103  1.00 16.66
ATOM    809  CA  ALA C 106      68.130  16.617   4.865  1.00 16.75
ATOM    810  C   ALA C 106      69.506  17.196   5.121  1.00 15.84
ATOM    811  O   ALA C 106      69.621  18.358   5.520  1.00 16.27
ATOM    812  CB  ALA C 106      67.469  17.246   3.645  1.00 17.32
ATOM    813  N   TYR C 107      70.558  16.390   4.881  1.00 15.99
ATOM    814  CA  TYR C 107      71.941  16.745   5.089  1.00 15.93
ATOM    815  C   TYR C 107      72.620  17.003   3.740  1.00 18.71
ATOM    816  O   TYR C 107      72.346  16.296   2.779  1.00 20.84
ATOM    817  CB  TYR C 107      72.714  15.637   5.835  1.00 19.26
ATOM    818  CG  TYR C 107      72.177  15.391   7.253  1.00 21.14
ATOM    819  CD1 TYR C 107      72.619  16.143   8.296  1.00 21.91
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ATOM	820	CD2	TYR	C	107	71.259	14.405	7.479	1.00	23.16
ATOM	821	CE1	TYR	C	107	72.125	15.931	9.596	1.00	24.59
ATOM	822	CE2	TYR	C	107	70.758	14.193	8.779	1.00	24.09
ATOM	823	CZ	TYR	C	107	71.220	14.964	9.794	1.00	27.50
ATOM	824	OH	TYR	C	107	70.760	14.801	11.101	1.00	29.66
ATOM	825	N	PHE	C	108	73.461	18.022	3.744	1.00	15.42
ATOM	826	CA	PHE	C	108	74.165	18.434	2.489	1.00	15.71
ATOM	827	C	PHE	C	108	75.646	18.525	2.624	1.00	19.91
ATOM	828	O	PHE	C	108	76.239	18.645	3.715	1.00	19.12
ATOM	829	CB	PHE	C	108	73.644	19.803	2.063	1.00	16.87
ATOM	830	CG	PHE	C	108	72.225	19.796	1.661	1.00	16.76
ATOM	831	CD1	PHE	C	108	71.195	19.910	2.626	1.00	17.17
ATOM	832	CD2	PHE	C	108	71.832	19.656	0.305	1.00	17.45
ATOM	833	CE1	PHE	C	108	69.873	19.871	2.240	1.00	19.62
ATOM	834	CE2	PHE	C	108	70.497	19.620	-0.081	1.00	20.41
ATOM	835	CZ	PHE	C	108	69.480	19.741	0.885	1.00	19.54
ATOM	836	N	GLU	C	109	76.311	18.516	1.444	1.00	17.02
ATOM	837	CA	GLU	C	109	77.762	18.671	1.404	1.00	17.21
ATOM	838	C	GLU	C	109	78.099	19.064	-0.072	1.00	15.89
ATOM	839	O	GLU	C	109	77.219	18.996	-0.910	1.00	16.10
ATOM	840	CB	GLU	C	109	78.483	17.338	1.695	1.00	18.77
ATOM	841	CG	GLU	C	109	78.226	16.303	0.620	1.00	19.64
ATOM	842	CD	GLU	C	109	78.915	14.936	0.838	1.00	21.63
ATOM	843	OE1	GLU	C	109	79.866	14.811	1.621	1.00	24.76
ATOM	844	OE2	GLU	C	109	78.472	13.999	0.170	1.00	28.24
ATOM	845	N	GLY	C	110	79.348	19.435	-0.277	1.00	15.85
ATOM	846	CA	GLY	C	110	79.829	19.789	-1.680	1.00	17.20
ATOM	847	C	GLY	C	110	78.950	20.810	-2.378	1.00	16.93
ATOM	848	O	GLY	C	110	78.634	21.885	-1.812	1.00	16.26
ATOM	849	N	ASP	C	111	78.534	20.528	-3.637	1.00	14.38
ATOM	850	CA	ASP	C	111	77.715	21.472	-4.391	1.00	14.84
ATOM	851	C	ASP	C	111	76.244	21.321	-4.079	1.00	14.72
ATOM	852	O	ASP	C	111	75.360	21.023	-4.904	1.00	14.34
ATOM	853	CB	ASP	C	111	77.999	21.194	-5.903	1.00	17.05
ATOM	854	CG	ASP	C	111	77.264	22.145	-6.828	1.00	19.59
ATOM	855	OD1	ASP	C	111	77.013	23.323	-6.491	1.00	20.52
ATOM	856	OD2	ASP	C	111	76.873	21.686	-7.928	1.00	19.81
ATOM	857	N	ASN	C	112	75.927	21.537	-2.787	1.00	14.68
ATOM	858	CA	ASN	C	112	74.503	21.373	-2.371	1.00	16.14
ATOM	859	C	ASN	C	112	73.952	19.992	-2.783	1.00	13.02
ATOM	860	O	ASN	C	112	72.799	19.870	-3.263	1.00	14.89
ATOM	861	CB	ASN	C	112	73.566	22.559	-2.717	1.00	16.17
ATOM	862	CG	ASN	C	112	73.880	23.786	-1.870	1.00	18.78
ATOM	863	OD1	ASN	C	112	74.533	23.641	-0.819	1.00	17.25
ATOM	864	ND2	ASN	C	112	73.429	24.960	-2.293	1.00	15.61
ATOM	865	N	GLU	C	113	74.785	18.960	-2.531	1.00	14.05
ATOM	866	CA	GLU	C	113	74.443	17.571	-2.819	1.00	15.74
ATOM	867	C	GLU	C	113	73.805	16.971	-1.563	1.00	18.95
ATOM	868	O	GLU	C	113	74.464	16.870	-0.539	1.00	19.58
ATOM	869	CB	GLU	C	113	75.708	16.797	-3.166	1.00	17.38
ATOM	870	CG	GLU	C	113	75.440	15.371	-3.668	1.00	20.91
ATOM	871	CD	GLU	C	113	74.661	15.313	-5.016	1.00	24.09
ATOM	872	OE1	GLU	C	113	75.023	15.987	-5.993	1.00	30.10
ATOM	873	OE2	GLU	C	113	73.680	14.559	-5.076	1.00	36.71
ATOM	874	N	MET	C	114	72.556	16.563	-1.684	1.00	18.64
ATOM	875	CA	MET	C	114	71.826	15.984	-0.519	1.00	20.88
ATOM	876	C	MET	C	114	72.331	14.600	-0.242	1.00	27.67
ATOM	877	O	MET	C	114	72.346	13.758	-1.144	1.00	27.90
ATOM	878	CB	MET	C	114	70.329	15.964	-0.798	1.00	23.89
ATOM	879	CG	MET	C	114	69.486	15.506	0.441	1.00	26.69

ATOM	880	SD	MET	C	114	67.734	15.561	0.136	1.00	29.33
ATOM	881	CE	MET	C	114	67.568	17.266	-0.315	1.00	23.75
ATOM	882	N	LYS	C	115	72.758	14.329	0.997	1.00	25.26
ATOM	883	CA	LYS	C	115	73.254	12.995	1.346	1.00	30.27
ATOM	884	C	LYS	C	115	72.131	11.966	1.381	1.00	36.08
ATOM	885	O	LYS	C	115	72.449	10.760	1.181	1.00	41.29
ATOM	886	CB	LYS	C	115	74.009	12.984	2.674	1.00	31.52
ATOM	887	CG	LYS	C	115	75.147	13.960	2.791	1.00	29.39
ATOM	888	CD	LYS	C	115	75.948	13.688	4.076	1.00	35.11
ATOM	889	CE	LYS	C	115	76.864	14.835	4.435	1.00	39.16
ATOM	890	NZ	LYS	C	115	77.861	14.448	5.498	1.00	41.83
ATOM	892	N	MET	D	1	41.087	33.198	23.825	1.00	17.87
ATOM	893	CA	MET	D	1	42.349	33.385	23.112	1.00	15.77
ATOM	894	C	MET	D	1	43.435	32.503	23.658	1.00	18.38
ATOM	895	O	MET	D	1	43.248	31.921	24.772	1.00	16.03
ATOM	896	CB	MET	D	1	42.724	34.805	22.826	1.00	18.15
ATOM	897	CG	MET	D	1	42.641	35.784	23.928	1.00	21.69
ATOM	898	SD	MET	D	1	43.800	35.292	25.234	1.00	24.50
ATOM	899	CE	MET	D	1	43.405	36.711	26.530	1.00	19.90
ATOM	900	N	ILE	D	2	44.516	32.347	22.912	1.00	13.90
ATOM	901	CA	ILE	D	2	45.595	31.431	23.276	1.00	12.73
ATOM	902	C	ILE	D	2	46.834	32.154	23.717	1.00	15.11
ATOM	903	O	ILE	D	2	47.335	33.086	23.088	1.00	13.08
ATOM	904	CB	ILE	D	2	45.916	30.531	22.029	1.00	12.91
ATOM	905	CG1	ILE	D	2	44.663	29.775	21.519	1.00	14.95
ATOM	906	CG2	ILE	D	2	47.077	29.650	22.239	1.00	13.31
ATOM	907	CD1	ILE	D	2	44.172	28.701	22.510	1.00	19.87
ATOM	908	N	ARG	D	3	47.332	31.720	24.876	1.00	11.64
ATOM	909	CA	ARG	D	3	48.516	32.296	25.459	1.00	9.38
ATOM	910	C	ARG	D	3	49.789	31.470	25.262	1.00	8.16
ATOM	911	O	ARG	D	3	49.708	30.234	25.113	1.00	9.82
ATOM	912	CB	ARG	D	3	48.295	32.255	27.026	1.00	11.91
ATOM	913	CG	ARG	D	3	47.131	33.118	27.499	1.00	12.07
ATOM	914	CD	ARG	D	3	47.529	34.571	27.783	1.00	12.41
ATOM	915	NE	ARG	D	3	46.447	35.256	28.452	1.00	12.53
ATOM	916	CZ	ARG	D	3	46.473	36.522	28.885	1.00	11.34
ATOM	917	NH1	ARG	D	3	47.517	37.336	28.661	1.00	11.49
ATOM	918	NH2	ARG	D	3	45.422	36.991	29.619	1.00	11.64
ATOM	919	N	THR	D	4	50.948	32.149	25.285	1.00	11.35
ATOM	920	CA	THR	D	4	52.272	31.500	25.210	1.00	10.99
ATOM	921	C	THR	D	4	52.813	31.593	26.693	1.00	9.80
ATOM	922	O	THR	D	4	52.986	32.672	27.155	1.00	10.46
ATOM	923	CB	THR	D	4	53.199	32.217	24.279	1.00	13.30
ATOM	924	OG1	THR	D	4	52.577	32.164	22.960	1.00	12.86
ATOM	925	CG2	THR	D	4	54.531	31.558	24.193	1.00	11.07
ATOM	926	N	MET	D	5	53.090	30.427	27.261	1.00	10.61
ATOM	927	CA	MET	D	5	53.555	30.329	28.694	1.00	10.17
ATOM	928	C	MET	D	5	54.837	29.563	28.799	1.00	13.79
ATOM	929	O	MET	D	5	55.101	28.614	28.027	1.00	12.14
ATOM	930	CB	MET	D	5	52.484	29.509	29.395	1.00	10.85
ATOM	931	CG	MET	D	5	51.061	30.164	29.397	1.00	13.35
ATOM	932	SD	MET	D	5	50.866	31.757	29.993	1.00	12.31
ATOM	933	CE	MET	D	5	51.031	31.458	31.862	1.00	9.06
ATOM	934	N	LEU	D	6	55.629	29.894	29.847	1.00	11.48
ATOM	935	CA	LEU	D	6	56.867	29.146	30.088	1.00	11.70
ATOM	936	C	LEU	D	6	56.504	27.682	30.442	1.00	15.58
ATOM	937	O	LEU	D	6	55.730	27.429	31.410	1.00	12.84
ATOM	938	CB	LEU	D	6	57.607	29.780	31.270	1.00	11.07
ATOM	939	CG	LEU	D	6	58.862	29.016	31.645	1.00	10.79
ATOM	940	CD1	LEU	D	6	60.065	29.206	30.628	1.00	12.32

ATOM	941	CD2	LEU	D	6	59.389	29.481	33.038	1.00	12.20
ATOM	942	N	GLN	D	7	56.980	26.693	29.671	1.00	11.50
ATOM	943	CA	GLN	D	7	56.694	25.319	29.932	1.00	12.08
ATOM	944	C	GLN	D	7	57.654	24.774	31.014	1.00	13.00
ATOM	945	O	GLN	D	7	57.222	23.966	31.908	1.00	13.76
ATOM	946	CB	GLN	D	7	56.889	24.443	28.642	1.00	13.70
ATOM	947	CG	GLN	D	7	56.481	23.024	28.769	1.00	13.52
ATOM	948	CD	GLN	D	7	57.490	22.096	29.530	1.00	15.62
ATOM	949	OE1	GLN	D	7	57.020	21.129	30.233	1.00	14.96
ATOM	950	NE2	GLN	D	7	58.822	22.323	29.355	1.00	13.51
ATOM	951	N	GLY	D	8	58.908	25.149	30.936	1.00	12.82
ATOM	952	CA	GLY	D	8	59.924	24.658	31.879	1.00	13.57
ATOM	953	C	GLY	D	8	61.276	25.264	31.576	1.00	17.33
ATOM	954	O	GLY	D	8	61.489	25.874	30.508	1.00	16.12
ATOM	955	N	LYS	D	9	62.225	25.176	32.515	1.00	13.73
ATOM	956	CA	LYS	D	9	63.535	25.722	32.269	1.00	14.09
ATOM	957	C	LYS	D	9	64.594	25.035	33.093	1.00	17.41
ATOM	958	O	LYS	D	9	64.293	24.412	34.150	1.00	16.23
ATOM	959	CB	LYS	D	9	63.604	27.197	32.448	1.00	17.25
ATOM	960	CG	LYS	D	9	63.491	27.641	33.937	1.00	16.41
ATOM	961	CD	LYS	D	9	63.860	29.094	34.196	1.00	16.11
ATOM	962	CE	LYS	D	9	63.661	29.538	35.703	1.00	20.64
ATOM	963	NZ	LYS	D	9	64.168	30.899	36.005	1.00	24.09
ATOM	964	N	LEU	D	10	65.795	25.085	32.580	1.00	14.37
ATOM	965	CA	LEU	D	10	67.019	24.574	33.245	1.00	13.07
ATOM	966	C	LEU	D	10	67.683	25.889	33.669	1.00	17.74
ATOM	967	O	LEU	D	10	68.139	26.719	32.864	1.00	15.88
ATOM	968	CB	LEU	D	10	67.917	23.753	32.313	1.00	12.64
ATOM	969	CG	LEU	D	10	67.275	22.500	31.721	1.00	16.69
ATOM	970	CD1	LEU	D	10	68.212	21.782	30.736	1.00	19.95
ATOM	971	CD2	LEU	D	10	66.799	21.474	32.834	1.00	18.21
ATOM	972	N	HIS	D	11	67.720	26.177	34.991	1.00	15.41
ATOM	973	CA	HIS	D	11	68.251	27.395	35.444	1.00	15.54
ATOM	974	C	HIS	D	11	69.702	27.368	35.893	1.00	20.36
ATOM	975	O	HIS	D	11	70.031	26.640	36.895	1.00	19.27
ATOM	976	CB	HIS	D	11	67.374	27.904	36.683	1.00	17.02
ATOM	977	CG	HIS	D	11	67.650	29.324	37.063	1.00	20.52
ATOM	978	ND1	HIS	D	11	67.137	30.393	36.361	1.00	23.10
ATOM	979	CD2	HIS	D	11	68.415	29.858	38.051	1.00	23.01
ATOM	980	CE1	HIS	D	11	67.563	31.524	36.895	1.00	22.29
ATOM	981	NE2	HIS	D	11	68.348	31.225	37.927	1.00	22.03
ATOM	982	N	ARG	D	12	70.556	28.124	35.209	1.00	17.66
ATOM	983	CA	ARG	D	12	71.956	28.229	35.513	1.00	17.87
ATOM	984	C	ARG	D	12	72.781	26.977	35.325	1.00	21.36
ATOM	985	O	ARG	D	12	73.632	26.605	36.187	1.00	21.72
ATOM	986	CB	ARG	D	12	72.232	28.945	36.891	1.00	17.27
ATOM	987	CG	ARG	D	12	71.708	30.362	36.941	1.00	16.85
ATOM	988	CD	ARG	D	12	71.907	31.054	38.323	1.00	21.64
ATOM	989	NE	ARG	D	12	73.332	31.030	38.693	1.00	26.91
ATOM	990	CZ	ARG	D	12	74.195	32.006	38.428	1.00	32.28
ATOM	991	NH1	ARG	D	12	75.471	31.878	38.797	1.00	32.70
ATOM	992	NH2	ARG	D	12	73.806	33.103	37.801	1.00	23.04
ATOM	993	N	VAL	D	13	72.613	26.297	34.173	1.00	16.36
ATOM	994	CA	VAL	D	13	73.413	25.135	33.867	1.00	16.81
ATOM	995	C	VAL	D	13	74.664	25.673	33.161	1.00	19.79
ATOM	996	O	VAL	D	13	74.668	26.811	32.683	1.00	21.56
ATOM	997	CB	VAL	D	13	72.713	24.137	32.918	1.00	20.87
ATOM	998	CG1	VAL	D	13	71.653	23.427	33.553	1.00	22.00
ATOM	999	CG2	VAL	D	13	72.189	24.846	31.612	1.00	19.93
ATOM	1000	N	LYS	D	14	75.741	24.892	33.128	1.00	17.58

ATOM	1001	CA	LYS	D	14	76.956	25.383	32.473	1.00	18.29
ATOM	1002	C	LYS	D	14	77.225	24.642	31.155	1.00	17.32
ATOM	1003	O	LYS	D	14	77.005	23.448	31.066	1.00	17.18
ATOM	1004	CB	LYS	D	14	78.176	25.251	33.416	1.00	21.96
ATOM	1005	CG	LYS	D	14	78.220	26.346	34.459	1.00	29.69
ATOM	1006	CD	LYS	D	14	79.441	26.161	35.412	1.00	27.98
ATOM	1007	CE	LYS	D	14	79.422	27.179	36.555	1.00	33.09
ATOM	1008	NZ	LYS	D	14	78.560	26.719	37.687	1.00	36.70
ATOM	1009	N	VAL	D	15	77.658	25.409	30.145	1.00	17.61
ATOM	1010	CA	VAL	D	15	77.967	24.799	28.844	1.00	15.98
ATOM	1011	C	VAL	D	15	79.203	23.888	29.035	1.00	18.36
ATOM	1012	O	VAL	D	15	80.185	24.318	29.603	1.00	20.10
ATOM	1013	CB	VAL	D	15	78.245	25.880	27.800	1.00	18.17
ATOM	1014	CG1	VAL	D	15	78.696	25.198	26.454	1.00	19.48
ATOM	1015	CG2	VAL	D	15	76.933	26.685	27.567	1.00	18.97
ATOM	1016	N	THR	D	16	79.140	22.659	28.545	1.00	16.59
ATOM	1017	CA	THR	D	16	80.271	21.721	28.715	1.00	18.46
ATOM	1018	C	THR	D	16	81.039	21.407	27.449	1.00	23.98
ATOM	1019	O	THR	D	16	82.184	20.892	27.500	1.00	23.98
ATOM	1020	CB	THR	D	16	79.781	20.374	29.348	1.00	20.68
ATOM	1021	OG1	THR	D	16	78.894	19.683	28.464	1.00	20.66
ATOM	1022	CG2	THR	D	16	79.048	20.647	30.719	1.00	20.82
ATOM	1023	N	HIS	D	17	80.447	21.718	26.302	1.00	21.79
ATOM	1024	CA	HIS	D	17	81.112	21.413	25.010	1.00	23.09
ATOM	1025	C	HIS	D	17	80.522	22.305	23.934	1.00	25.64
ATOM	1026	O	HIS	D	17	79.371	22.760	24.047	1.00	20.59
ATOM	1027	CB	HIS	D	17	80.740	19.928	24.685	1.00	25.73
ATOM	1028	CG	HIS	D	17	81.356	19.348	23.433	1.00	31.57
ATOM	1029	ND1	HIS	D	17	80.584	18.824	22.407	1.00	34.88
ATOM	1030	CD2	HIS	D	17	82.652	19.158	23.062	1.00	34.96
ATOM	1031	CE1	HIS	D	17	81.374	18.360	21.451	1.00	35.01
ATOM	1032	NE2	HIS	D	17	82.635	18.549	21.820	1.00	35.08
ATOM	1033	N	ALA	D	18	81.309	22.554	22.893	1.00	25.07
ATOM	1034	CA	ALA	D	18	80.848	23.379	21.759	1.00	25.93
ATOM	1035	C	ALA	D	18	81.317	22.603	20.501	1.00	31.11
ATOM	1036	O	ALA	D	18	82.460	22.106	20.472	1.00	33.50
ATOM	1037	CB	ALA	D	18	81.433	24.755	21.814	1.00	27.54
ATOM	1038	N	ASP	D	19	80.444	22.423	19.505	1.00	24.42
ATOM	1039	CA	ASP	D	19	80.814	21.654	18.284	1.00	24.78
ATOM	1040	C	ASP	D	19	80.276	22.359	17.047	1.00	27.05
ATOM	1041	O	ASP	D	19	79.206	22.000	16.529	1.00	24.71
ATOM	1042	CB	ASP	D	19	80.272	20.218	18.402	1.00	25.96
ATOM	1043	CG	ASP	D	19	80.644	19.316	17.214	1.00	34.10
ATOM	1044	OD1	ASP	D	19	81.404	19.749	16.320	1.00	34.04
ATOM	1045	OD2	ASP	D	19	80.164	18.147	17.193	1.00	38.22
ATOM	1046	N	LEU	D	20	81.027	23.356	16.587	1.00	25.80
ATOM	1047	CA	LEU	D	20	80.656	24.143	15.422	1.00	24.85
ATOM	1048	C	LEU	D	20	80.390	23.317	14.170	1.00	27.59
ATOM	1049	O	LEU	D	20	79.410	23.581	13.451	1.00	26.06
ATOM	1050	CB	LEU	D	20	81.753	25.185	15.120	1.00	25.72
ATOM	1051	CG	LEU	D	20	81.546	26.193	13.977	1.00	29.24
ATOM	1052	CD1	LEU	D	20	80.505	27.239	14.355	1.00	28.84
ATOM	1053	CD2	LEU	D	20	82.887	26.875	13.627	1.00	29.15
ATOM	1054	N	HIS	D	21	81.264	22.340	13.908	1.00	28.61
ATOM	1055	CA	HIS	D	21	81.167	21.442	12.712	1.00	30.90
ATOM	1056	C	HIS	D	21	80.238	20.275	12.779	1.00	36.12
ATOM	1057	O	HIS	D	21	80.249	19.385	11.890	1.00	35.00
ATOM	1058	CB	HIS	D	21	82.573	21.039	12.237	1.00	32.76
ATOM	1059	CG	HIS	D	21	83.437	22.204	11.941	1.00	36.81
ATOM	1060	ND1	HIS	D	21	84.537	22.541	12.700	1.00	39.48

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ATOM   1061  CD2 HIS D  21      83.307  23.181  11.010  1.00 38.76
ATOM   1062  CE1 HIS D  21      85.072  23.656  12.222  1.00 38.26
ATOM   1063  NE2 HIS D  21      84.345  24.063  11.198  1.00 38.36
ATOM   1064  N   TYR D  22      79.418  20.275  13.811  1.00 33.13
ATOM   1065  CA  TYR D  22      78.453  19.220  14.019  1.00 33.14
ATOM   1066  C   TYR D  22      77.573  18.876  12.801  1.00 37.60
ATOM   1067  O   TYR D  22      77.155  19.766  12.012  1.00 32.76
ATOM   1068  CB  TYR D  22      77.479  19.691  15.105  1.00 33.35
ATOM   1069  CG  TYR D  22      76.571  18.617  15.617  1.00 35.03
ATOM   1070  CD1 TYR D  22      77.095  17.527  16.305  1.00 36.82
ATOM   1071  CD2 TYR D  22      75.204  18.670  15.401  1.00 35.58
ATOM   1072  CE1 TYR D  22      76.271  16.517  16.773  1.00 37.35
ATOM   1073  CE2 TYR D  22      74.375  17.669  15.872  1.00 36.01
ATOM   1074  CZ  TYR D  22      74.906  16.604  16.557  1.00 42.70
ATOM   1075  OH  TYR D  22      74.016  15.625  17.014  1.00 46.65
ATOM   1076  N   GLU D  23      77.276  17.594  12.694  1.00 39.24
ATOM   1077  CA  GLU D  23      76.408  17.072  11.664  1.00 42.44
ATOM   1078  C   GLU D  23      75.374  16.147  12.358  1.00 47.01
ATOM   1079  O   GLU D  23      75.698  15.050  12.769  1.00 48.53
ATOM   1080  CB  GLU D  23      77.176  16.320  10.575  1.00 44.81
ATOM   1081  CG  GLU D  23      76.241  15.586   9.631  1.00 53.00
ATOM   1082  CD  GLU D  23      76.852  15.314   8.271  1.00 63.57
ATOM   1083  OE1 GLU D  23      78.097  15.153   8.190  1.00 70.57
ATOM   1084  OE2 GLU D  23      76.079  15.237   7.285  1.00 49.95
ATOM   1085  N   GLY D  24      74.136  16.608  12.481  1.00 43.35
ATOM   1086  CA  GLY D  24      73.103  15.797  13.108  1.00 47.63
ATOM   1087  C   GLY D  24      71.872  16.608  13.529  1.00 49.81
ATOM   1088  O   GLY D  24      71.438  17.481  12.758  1.00 43.71
ATOM   1089  OH  GLY D  24      71.339  16.374  14.643  1.00 78.26
ATOM   1090  C   PVL D  25      72.100  22.561  19.543  1.00 18.29
ATOM   1091  O   PVL D  25      73.123  23.121  19.763  1.00 21.21
ATOM   1092  CA  PVL D  25      71.565  22.581  18.161  1.00 27.46
ATOM   1093  CB  PVL D  25      70.223  21.973  17.952  1.00 25.35
ATOM   1094  ON  PVL D  25      72.196  23.134  17.245  1.00 33.71
ATOM   1095  N   CYS D  26      71.286  22.044  20.569  1.00 15.60
ATOM   1096  CA  CYS D  26      71.834  22.016  21.931  1.00 16.64
ATOM   1097  CB  CYS D  26      71.304  23.212  22.757  1.00 14.30
ATOM   1098  SG  CYS D  26      71.996  23.106  24.461  1.00 18.05
ATOM   1099  C   CYS D  26      71.504  20.649  22.505  1.00 14.55
ATOM   1100  O   CYS D  26      70.332  20.263  22.665  1.00 16.28
ATOM   1101  N   ALA D  27      72.569  19.844  22.774  1.00 15.46
ATOM   1102  CA  ALA D  27      72.411  18.463  23.329  1.00 15.63
ATOM   1103  C   ALA D  27      72.469  18.581  24.869  1.00 15.10
ATOM   1104  O   ALA D  27      73.350  19.198  25.406  1.00 15.77
ATOM   1105  CB  ALA D  27      73.510  17.508  22.838  1.00 16.71
ATOM   1106  N   ILE D  28      71.483  17.965  25.486  1.00 14.23
ATOM   1107  CA  ILE D  28      71.292  18.058  26.940  1.00 14.71
ATOM   1108  C   ILE D  28      71.023  16.715  27.562  1.00 17.41
ATOM   1109  O   ILE D  28      70.251  15.919  27.072  1.00 16.90
ATOM   1110  CB  ILE D  28      69.990  18.945  27.121  1.00 16.58
ATOM   1111  CG1 ILE D  28      70.204  20.317  26.472  1.00 16.36
ATOM   1112  CG2 ILE D  28      69.627  19.068  28.632  1.00 15.52
ATOM   1113  CD1 ILE D  28      68.887  21.088  26.119  1.00 18.68
ATOM   1114  N   ASP D  29      71.717  16.475  28.696  1.00 16.97
ATOM   1115  CA  ASP D  29      71.551  15.203  29.449  1.00 18.01
ATOM   1116  C   ASP D  29      70.023  14.912  29.600  1.00 17.51
ATOM   1117  O   ASP D  29      69.284  15.814  30.061  1.00 15.93
ATOM   1118  CB  ASP D  29      72.168  15.468  30.837  1.00 18.64
ATOM   1119  CG  ASP D  29      72.085  14.248  31.826  1.00 21.55
ATOM   1120  OD1 ASP D  29      71.218  13.349  31.704  1.00 21.30
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ATOM   1121  OD2 ASP D  29      72.956  14.262  32.752  1.00 22.85
ATOM   1122  N   GLN D  30      69.580  13.710  29.207  1.00 17.64
ATOM   1123  CA  GLN D  30      68.165  13.289  29.288  1.00 16.64
ATOM   1124  C   GLN D  30      67.584  13.514  30.685  1.00 20.42
ATOM   1125  O   GLN D  30      66.407  13.865  30.795  1.00 19.64
ATOM   1126  CB  GLN D  30      67.942  11.845  28.839  1.00 19.10
ATOM   1127  CG  GLN D  30      66.498  11.417  28.796  1.00 20.18
ATOM   1128  CD  GLN D  30      65.710  12.200  27.766  1.00 24.27
ATOM   1129  OE1 GLN D  30      66.090  12.214  26.565  1.00 20.83
ATOM   1130  NE2 GLN D  30      64.598  12.837  28.202  1.00 20.72
ATOM   1131  N   ASP D  31      68.383  13.362  31.752  1.00 19.98
ATOM   1132  CA  ASP D  31      67.810  13.608  33.086  1.00 20.52
ATOM   1133  C   ASP D  31      67.343  15.055  33.267  1.00 19.87
ATOM   1134  O   ASP D  31      66.339  15.342  34.003  1.00 20.49
ATOM   1135  CB  ASP D  31      68.858  13.326  34.165  1.00 20.56
ATOM   1136  CG  ASP D  31      68.955  11.861  34.505  1.00 27.59
ATOM   1137  OD1 ASP D  31      68.027  11.063  34.248  1.00 27.63
ATOM   1138  OD2 ASP D  31      70.061  11.498  34.988  1.00 25.47
ATOM   1139  N   PHE D  32      68.053  16.002  32.616  1.00 17.26
ATOM   1140  CA  PHE D  32      67.743  17.411  32.698  1.00 16.13
ATOM   1141  C   PHE D  32      66.457  17.661  31.896  1.00 15.84
ATOM   1142  O   PHE D  32      65.527  18.389  32.356  1.00 15.43
ATOM   1143  CB  PHE D  32      68.854  18.301  32.116  1.00 17.62
ATOM   1144  CG  PHE D  32      70.216  18.172  32.810  1.00 18.64
ATOM   1145  CD1 PHE D  32      70.409  17.355  33.944  1.00 20.38
ATOM   1146  CD2 PHE D  32      71.294  18.902  32.313  1.00 21.28
ATOM   1147  CE1 PHE D  32      71.722  17.281  34.537  1.00 21.62
ATOM   1148  CE2 PHE D  32      72.549  18.834  32.878  1.00 24.06
ATOM   1149  CZ  PHE D  32      72.763  18.019  34.007  1.00 22.14
ATOM   1150  N   LEU D  33      66.412  17.068  30.700  1.00 15.62
ATOM   1151  CA  LEU D  33      65.206  17.230  29.867  1.00 15.62
ATOM   1152  C   LEU D  33      63.969  16.737  30.662  1.00 14.56
ATOM   1153  O   LEU D  33      62.938  17.393  30.680  1.00 15.50
ATOM   1154  CB  LEU D  33      65.330  16.434  28.565  1.00 15.46
ATOM   1155  CG  LEU D  33      66.446  16.945  27.597  1.00 17.68
ATOM   1156  CD1 LEU D  33      66.471  16.024  26.336  1.00 18.11
ATOM   1157  CD2 LEU D  33      66.139  18.385  27.159  1.00 17.59
ATOM   1158  N   ASP D  34      64.094  15.567  31.320  1.00 15.47
ATOM   1159  CA  ASP D  34      63.010  14.958  32.091  1.00 15.42
ATOM   1160  C   ASP D  34      62.498  15.897  33.177  1.00 15.50
ATOM   1161  O   ASP D  34      61.312  16.032  33.342  1.00 16.94
ATOM   1162  CB  ASP D  34      63.523  13.673  32.755  1.00 16.78
ATOM   1163  CG  ASP D  34      63.625  12.511  31.796  1.00 21.53
ATOM   1164  OD1 ASP D  34      63.254  12.639  30.594  1.00 22.41
ATOM   1165  OD2 ASP D  34      64.107  11.419  32.237  1.00 24.39
ATOM   1166  N   ALA D  35      63.405  16.522  33.911  1.00 15.30
ATOM   1167  CA  ALA D  35      63.030  17.444  34.982  1.00 16.57
ATOM   1168  C   ALA D  35      62.344  18.711  34.497  1.00 18.73
ATOM   1169  O   ALA D  35      61.440  19.244  35.142  1.00 19.02
ATOM   1170  CB  ALA D  35      64.253  17.838  35.828  1.00 18.18
ATOM   1171  N   ALA D  36      62.814  19.231  33.338  1.00 15.77
ATOM   1172  CA  ALA D  36      62.243  20.432  32.837  1.00 14.01
ATOM   1173  C   ALA D  36      61.034  20.203  31.866  1.00 12.66
ATOM   1174  O   ALA D  36      60.427  21.243  31.459  1.00 15.97
ATOM   1175  CB  ALA D  36      63.337  21.261  32.105  1.00 15.98
ATOM   1176  N   GLY D  37      60.750  18.962  31.520  1.00 12.31
ATOM   1177  CA  GLY D  37      59.663  18.637  30.636  1.00 12.99
ATOM   1178  C   GLY D  37      59.994  19.050  29.180  1.00 13.99
ATOM   1179  O   GLY D  37      59.023  19.117  28.371  1.00 13.49
ATOM   1180  N   ILE D  38      61.276  19.246  28.882  1.00 13.30
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ATOM	1181	CA	ILE	D	38	61.705	19.641	27.476	1.00	11.90
ATOM	1182	C	ILE	D	38	61.854	18.372	26.665	1.00	13.73
ATOM	1183	O	ILE	D	38	62.470	17.403	27.086	1.00	13.87
ATOM	1184	CB	ILE	D	38	62.938	20.454	27.528	1.00	12.06
ATOM	1185	CG1	ILE	D	38	62.664	21.817	28.244	1.00	13.02
ATOM	1186	CG2	ILE	D	38	63.457	20.747	26.031	1.00	11.46
ATOM	1187	CD1	ILE	D	38	63.886	22.662	28.502	1.00	14.92
ATOM	1188	N	LEU	D	39	61.313	18.366	25.415	1.00	11.75
ATOM	1189	CA	LEU	D	39	61.366	17.198	24.557	1.00	11.57
ATOM	1190	C	LEU	D	39	62.445	17.286	23.489	1.00	13.60
ATOM	1191	O	LEU	D	39	62.811	18.368	23.105	1.00	12.83
ATOM	1192	CB	LEU	D	39	60.048	17.052	23.807	1.00	11.62
ATOM	1193	CG	LEU	D	39	58.724	17.113	24.610	1.00	13.66
ATOM	1194	CD1	LEU	D	39	57.552	16.938	23.682	1.00	15.79
ATOM	1195	CD2	LEU	D	39	58.820	15.969	25.666	1.00	15.29
ATOM	1196	N	GLU	D	40	62.956	16.134	23.119	1.00	14.52
ATOM	1197	CA	GLU	D	40	63.930	16.098	22.000	1.00	14.56
ATOM	1198	C	GLU	D	40	63.128	16.706	20.790	1.00	14.90
ATOM	1199	O	GLU	D	40	61.938	16.424	20.582	1.00	13.14
ATOM	1200	CB	GLU	D	40	64.273	14.643	21.690	1.00	17.43
ATOM	1201	CG	GLU	D	40	65.687	14.237	22.093	1.00	36.71
ATOM	1202	CD	GLU	D	40	66.336	13.346	21.016	1.00	43.99
ATOM	1203	OE1	GLU	D	40	65.691	12.317	20.674	1.00	33.64
ATOM	1204	OE2	GLU	D	40	67.475	13.665	20.501	1.00	23.74
ATOM	1205	N	ASN	D	41	63.849	17.563	20.028	1.00	12.38
ATOM	1206	CA	ASN	D	41	63.297	18.252	18.835	1.00	12.93
ATOM	1207	C	ASN	D	41	62.403	19.417	19.130	1.00	15.81
ATOM	1208	O	ASN	D	41	61.836	20.050	18.252	1.00	13.21
ATOM	1209	CB	ASN	D	41	62.680	17.270	17.864	1.00	14.28
ATOM	1210	CG	ASN	D	41	63.721	16.286	17.293	1.00	12.10
ATOM	1211	OD1	ASN	D	41	64.828	16.679	16.930	1.00	16.64
ATOM	1212	ND2	ASN	D	41	63.373	15.002	17.295	1.00	15.27
ATOM	1213	N	GLU	D	42	62.241	19.771	20.402	1.00	10.98
ATOM	1214	CA	GLU	D	42	61.432	20.916	20.753	1.00	9.74
ATOM	1215	C	GLU	D	42	62.214	22.225	20.638	1.00	9.74
ATOM	1216	O	GLU	D	42	63.430	22.297	20.917	1.00	10.17
ATOM	1217	CB	GLU	D	42	60.958	20.806	22.304	1.00	10.40
ATOM	1218	CG	GLU	D	42	59.992	21.930	22.730	1.00	10.03
ATOM	1219	CD	GLU	D	42	59.538	21.802	24.213	1.00	13.25
ATOM	1220	OE1	GLU	D	42	60.180	20.979	24.893	1.00	15.16
ATOM	1221	OE2	GLU	D	42	58.595	22.504	24.588	1.00	12.03
ATOM	1222	N	ALA	D	43	61.529	23.303	20.212	1.00	9.51
ATOM	1223	CA	ALA	D	43	62.125	24.618	20.139	1.00	10.88
ATOM	1224	C	ALA	D	43	62.581	25.062	21.572	1.00	10.85
ATOM	1225	O	ALA	D	43	61.770	24.882	22.523	1.00	11.54
ATOM	1226	CB	ALA	D	43	61.086	25.666	19.611	1.00	12.49
ATOM	1227	N	ILE	D	44	63.746	25.596	21.711	1.00	11.86
ATOM	1228	CA	ILE	D	44	64.214	26.108	23.049	1.00	11.02
ATOM	1229	C	ILE	D	44	64.876	27.495	22.885	1.00	13.51
ATOM	1230	O	ILE	D	44	65.459	27.820	21.790	1.00	13.63
ATOM	1231	CB	ILE	D	44	65.215	25.146	23.757	1.00	12.21
ATOM	1232	CG1	ILE	D	44	66.425	24.841	22.799	1.00	12.04
ATOM	1233	CG2	ILE	D	44	64.475	23.886	24.201	1.00	14.58
ATOM	1234	CD1	ILE	D	44	67.496	23.934	23.440	1.00	12.27
ATOM	1235	N	ASP	D	45	64.845	28.343	23.921	1.00	10.42
ATOM	1236	CA	ASP	D	45	65.470	29.634	23.942	1.00	10.06
ATOM	1237	C	ASP	D	45	66.628	29.457	24.943	1.00	14.23
ATOM	1238	O	ASP	D	45	66.438	28.814	26.014	1.00	14.99
ATOM	1239	CB	ASP	D	45	64.514	30.754	24.407	1.00	12.39
ATOM	1240	CG	ASP	D	45	63.320	30.886	23.509	1.00	15.51

ATOM	1241	OD1	ASP	D	45	63.504	30.682	22.250	1.00	15.80
ATOM	1242	OD2	ASP	D	45	62.187	31.118	23.974	1.00	15.67
ATOM	1243	N	ILE	D	46	67.791	29.995	24.634	1.00	10.63
ATOM	1244	CA	ILE	D	46	68.996	29.909	25.471	1.00	10.58
ATOM	1245	C	ILE	D	46	69.427	31.327	25.747	1.00	14.80
ATOM	1246	O	ILE	D	46	69.649	32.151	24.860	1.00	13.14
ATOM	1247	CB	ILE	D	46	70.104	29.079	24.805	1.00	12.68
ATOM	1248	CG1	ILE	D	46	69.560	27.686	24.519	1.00	11.97
ATOM	1249	CG2	ILE	D	46	71.354	29.057	25.751	1.00	14.01
ATOM	1250	CD1	ILE	D	46	70.647	26.680	24.071	1.00	17.51
ATOM	1251	N	TRP	D	47	69.509	31.672	27.067	1.00	11.09
ATOM	1252	CA	TRP	D	47	69.832	32.990	27.530	1.00	12.91
ATOM	1253	C	TRP	D	47	71.163	32.842	28.298	1.00	18.14
ATOM	1254	O	TRP	D	47	71.232	32.122	29.319	1.00	16.83
ATOM	1255	CB	TRP	D	47	68.681	33.497	28.446	1.00	12.75
ATOM	1256	CG	TRP	D	47	67.334	33.535	27.762	1.00	12.68
ATOM	1257	CD1	TRP	D	47	67.087	33.885	26.416	1.00	13.80
ATOM	1258	CD2	TRP	D	47	66.070	33.224	28.316	1.00	12.97
ATOM	1259	NE1	TRP	D	47	65.765	33.773	26.151	1.00	12.97
ATOM	1260	CE2	TRP	D	47	65.093	33.372	27.286	1.00	14.42
ATOM	1261	CE3	TRP	D	47	65.650	32.757	29.579	1.00	14.96
ATOM	1262	CZ2	TRP	D	47	63.744	33.139	27.488	1.00	14.53
ATOM	1263	CZ3	TRP	D	47	64.331	32.544	29.792	1.00	16.02
ATOM	1264	CH2	TRP	D	47	63.365	32.734	28.774	1.00	16.49
ATOM	1265	N	ASN	D	48	72.217	33.452	27.762	1.00	15.37
ATOM	1266	CA	ASN	D	48	73.574	33.323	28.320	1.00	15.56
ATOM	1267	C	ASN	D	48	73.829	34.347	29.393	1.00	16.84
ATOM	1268	O	ASN	D	48	73.955	35.526	29.124	1.00	15.08
ATOM	1269	CB	ASN	D	48	74.577	33.489	27.132	1.00	14.22
ATOM	1270	CG	ASN	D	48	75.962	33.037	27.477	1.00	19.83
ATOM	1271	OD1	ASN	D	48	76.445	33.343	28.575	1.00	17.68
ATOM	1272	ND2	ASN	D	48	76.625	32.305	26.581	1.00	18.60
ATOM	1273	N	VAL	D	49	73.892	33.883	30.661	1.00	16.35
ATOM	1274	CA	VAL	D	49	74.128	34.782	31.784	1.00	16.91
ATOM	1275	C	VAL	D	49	75.563	35.373	31.784	1.00	18.54
ATOM	1276	O	VAL	D	49	75.809	36.526	32.220	1.00	19.45
ATOM	1277	CB	VAL	D	49	73.926	34.037	33.092	1.00	20.06
ATOM	1278	CG1	VAL	D	49	74.124	35.006	34.262	1.00	21.67
ATOM	1279	CG2	VAL	D	49	72.526	33.407	33.136	1.00	18.68
ATOM	1280	N	THR	D	50	76.501	34.576	31.282	1.00	17.72
ATOM	1281	CA	THR	D	50	77.881	35.042	31.234	1.00	18.92
ATOM	1282	C	THR	D	50	78.125	36.187	30.258	1.00	20.97
ATOM	1283	O	THR	D	50	78.696	37.231	30.614	1.00	20.06
ATOM	1284	CB	THR	D	50	78.829	33.887	30.935	1.00	19.40
ATOM	1285	OG1	THR	D	50	78.678	32.859	31.930	1.00	19.82
ATOM	1286	CG2	THR	D	50	80.335	34.365	30.836	1.00	21.30
ATOM	1287	N	ASN	D	51	77.687	36.000	28.998	1.00	17.46
ATOM	1288	CA	ASN	D	51	77.917	37.033	27.972	1.00	18.39
ATOM	1289	C	ASN	D	51	76.723	37.838	27.459	1.00	19.48
ATOM	1290	O	ASN	D	51	76.883	38.713	26.603	1.00	19.00
ATOM	1291	CB	ASN	D	51	78.712	36.436	26.788	1.00	18.51
ATOM	1292	CG	ASN	D	51	77.871	35.497	25.912	1.00	22.35
ATOM	1293	OD1	ASN	D	51	76.653	35.449	26.014	1.00	17.21
ATOM	1294	ND2	ASN	D	51	78.537	34.732	25.071	1.00	21.24
ATOM	1295	N	GLY	D	52	75.528	37.546	27.979	1.00	15.50
ATOM	1296	CA	GLY	D	52	74.286	38.204	27.622	1.00	14.95
ATOM	1297	C	GLY	D	52	73.637	37.851	26.263	1.00	14.04
ATOM	1298	O	GLY	D	52	72.553	38.408	25.971	1.00	16.62
ATOM	1299	N	LYS	D	53	74.271	36.968	25.507	1.00	14.08
ATOM	1300	CA	LYS	D	53	73.636	36.627	24.193	1.00	14.38

ATOM	1301	C	LYS	D	53	72.355	35.864	24.437	1.00	15.94
ATOM	1302	O	LYS	D	53	72.229	35.159	25.442	1.00	16.45
ATOM	1303	CB	LYS	D	53	74.596	35.808	23.323	1.00	14.22
ATOM	1304	CG	LYS	D	53	75.791	36.669	22.909	1.00	16.49
ATOM	1305	CD	LYS	D	53	76.764	35.880	22.038	1.00	19.28
ATOM	1306	CE	LYS	D	53	77.988	36.725	21.678	1.00	26.70
ATOM	1307	NZ	LYS	D	53	79.004	35.889	20.987	1.00	29.14
ATOM	1308	N	ARG	D	54	71.393	35.958	23.483	1.00	12.88
ATOM	1309	CA	ARG	D	54	70.123	35.274	23.557	1.00	11.93
ATOM	1310	C	ARG	D	54	69.855	34.669	22.194	1.00	14.91
ATOM	1311	O	ARG	D	54	69.980	35.396	21.196	1.00	15.98
ATOM	1312	CB	ARG	D	54	68.981	36.222	23.931	1.00	13.59
ATOM	1313	CG	ARG	D	54	69.328	37.048	25.222	1.00	14.24
ATOM	1314	CD	ARG	D	54	68.216	38.045	25.627	1.00	13.75
ATOM	1315	NE	ARG	D	54	67.011	37.440	26.165	1.00	13.94
ATOM	1316	CZ	ARG	D	54	66.877	37.091	27.456	1.00	16.69
ATOM	1317	NH1	ARG	D	54	67.936	37.309	28.276	1.00	13.80
ATOM	1318	NH2	ARG	D	54	65.726	36.552	27.929	1.00	13.52
ATOM	1319	N	PHE	D	55	69.566	33.396	22.152	1.00	12.40
ATOM	1320	CA	PHE	D	55	69.306	32.745	20.862	1.00	13.30
ATOM	1321	C	PHE	D	55	68.292	31.657	20.971	1.00	18.51
ATOM	1322	O	PHE	D	55	67.947	31.225	22.083	1.00	16.08
ATOM	1323	CB	PHE	D	55	70.609	32.327	20.200	1.00	13.02
ATOM	1324	CG	PHE	D	55	71.346	31.246	20.922	1.00	14.95
ATOM	1325	CD1	PHE	D	55	72.197	31.565	22.004	1.00	15.75
ATOM	1326	CD2	PHE	D	55	71.234	29.901	20.513	1.00	15.13
ATOM	1327	CE1	PHE	D	55	72.938	30.508	22.680	1.00	17.56
ATOM	1328	CE2	PHE	D	55	71.931	28.901	21.171	1.00	17.23
ATOM	1329	CZ	PHE	D	55	72.794	29.230	22.258	1.00	16.09
ATOM	1330	N	SER	D	56	67.760	31.175	19.846	1.00	12.78
ATOM	1331	CA	SER	D	56	66.764	30.135	19.824	1.00	12.18
ATOM	1332	C	SER	D	56	67.220	29.017	18.940	1.00	15.48
ATOM	1333	O	SER	D	56	67.772	29.295	17.870	1.00	14.26
ATOM	1334	CB	SER	D	56	65.408	30.618	19.392	1.00	13.68
ATOM	1335	OG	SER	D	56	64.906	31.668	20.254	1.00	18.10
ATOM	1336	N	THR	D	57	67.010	27.786	19.358	1.00	11.29
ATOM	1337	CA	THR	D	57	67.456	26.580	18.617	1.00	11.02
ATOM	1338	C	THR	D	57	66.477	25.422	18.955	1.00	11.10
ATOM	1339	O	THR	D	57	65.269	25.655	19.137	1.00	10.41
ATOM	1340	CB	THR	D	57	68.956	26.316	18.937	1.00	13.63
ATOM	1341	OG1	THR	D	57	69.406	25.158	18.211	1.00	16.82
ATOM	1342	CG2	THR	D	57	69.148	25.977	20.458	1.00	16.40
ATOM	1343	N	TYR	D	58	66.953	24.186	19.039	1.00	11.85
ATOM	1344	CA	TYR	D	58	66.081	23.039	19.381	1.00	11.66
ATOM	1345	C	TYR	D	58	66.898	22.079	20.219	1.00	14.10
ATOM	1346	O	TYR	D	58	68.132	22.085	20.147	1.00	12.80
ATOM	1347	CB	TYR	D	58	65.417	22.357	18.154	1.00	13.66
ATOM	1348	CG	TYR	D	58	66.346	21.598	17.249	1.00	14.03
ATOM	1349	CD1	TYR	D	58	67.006	22.243	16.175	1.00	14.60
ATOM	1350	CD2	TYR	D	58	66.578	20.259	17.424	1.00	14.69
ATOM	1351	CE1	TYR	D	58	67.879	21.541	15.366	1.00	14.59
ATOM	1352	CE2	TYR	D	58	67.453	19.534	16.587	1.00	16.85
ATOM	1353	CZ	TYR	D	58	68.099	20.201	15.564	1.00	21.58
ATOM	1354	OH	TYR	D	58	68.989	19.626	14.678	1.00	22.59
ATOM	1355	N	ALA	D	59	66.215	21.278	21.038	1.00	12.25
ATOM	1356	CA	ALA	D	59	66.907	20.349	21.895	1.00	12.10
ATOM	1357	C	ALA	D	59	67.209	19.007	21.292	1.00	14.08
ATOM	1358	O	ALA	D	59	66.420	18.450	20.545	1.00	13.85
ATOM	1359	CB	ALA	D	59	66.015	20.122	23.160	1.00	13.24
ATOM	1360	N	ILE	D	60	68.365	18.433	21.690	1.00	15.08

ATOM	1361	CA	ILE	D	60	68.803	17.122	21.272	1.00	17.01
ATOM	1362	C	ILE	D	60	69.125	16.356	22.591	1.00	16.03
ATOM	1363	O	ILE	D	60	69.663	16.961	23.500	1.00	16.17
ATOM	1364	CB	ILE	D	60	70.125	17.251	20.437	1.00	20.97
ATOM	1365	CG1	ILE	D	60	69.809	17.848	19.062	1.00	23.49
ATOM	1366	CG2	ILE	D	60	70.789	15.887	20.217	1.00	23.18
ATOM	1367	CD1	ILE	D	60	71.051	18.391	18.335	1.00	26.91
ATOM	1368	N	ALA	D	61	68.770	15.083	22.679	1.00	16.21
ATOM	1369	CA	ALA	D	61	69.073	14.329	23.908	1.00	17.99
ATOM	1370	C	ALA	D	61	70.540	13.922	23.939	1.00	20.83
ATOM	1371	O	ALA	D	61	71.084	13.484	22.911	1.00	20.99
ATOM	1372	CB	ALA	D	61	68.241	13.116	23.982	1.00	19.35
ATOM	1373	N	ALA	D	62	71.155	14.020	25.121	1.00	17.91
ATOM	1374	CA	ALA	D	62	72.553	13.581	25.379	1.00	17.67
ATOM	1375	C	ALA	D	62	72.369	12.443	26.406	1.00	23.91
ATOM	1376	O	ALA	D	62	71.329	12.319	27.041	1.00	22.36
ATOM	1377	CB	ALA	D	62	73.402	14.661	25.953	1.00	18.45
ATOM	1378	N	GLU	D	63	73.395	11.613	26.540	1.00	22.90
ATOM	1379	CA	GLU	D	63	73.378	10.471	27.428	1.00	23.71
ATOM	1380	C	GLU	D	63	72.950	10.793	28.843	1.00	23.19
ATOM	1381	O	GLU	D	63	73.447	11.742	29.441	1.00	22.01
ATOM	1382	CB	GLU	D	63	74.777	9.848	27.443	1.00	25.20
ATOM	1383	CG	GLU	D	63	74.859	8.627	28.342	1.00	31.69
ATOM	1384	CD	GLU	D	63	76.110	7.846	28.078	1.00	54.65
ATOM	1385	OE1	GLU	D	63	76.067	6.926	27.227	1.00	50.68
ATOM	1386	OE2	GLU	D	63	77.136	8.166	28.714	1.00	49.85
ATOM	1387	N	ARG	D	64	72.047	9.967	29.375	1.00	23.54
ATOM	1388	CA	ARG	D	64	71.554	10.144	30.721	1.00	24.49
ATOM	1389	C	ARG	D	64	72.710	10.059	31.727	1.00	29.91
ATOM	1390	O	ARG	D	64	73.501	9.102	31.685	1.00	30.10
ATOM	1391	CB	ARG	D	64	70.529	9.064	31.047	1.00	24.54
ATOM	1392	CG	ARG	D	64	69.732	9.364	32.284	1.00	33.44
ATOM	1393	CD	ARG	D	64	68.790	8.227	32.617	1.00	30.76
ATOM	1394	NE	ARG	D	64	67.706	8.048	31.659	1.00	27.92
ATOM	1395	CZ	ARG	D	64	66.649	8.865	31.545	1.00	30.52
ATOM	1396	NH1	ARG	D	64	66.536	9.940	32.316	1.00	26.37
ATOM	1397	NH2	ARG	D	64	65.710	8.597	30.655	1.00	30.42
ATOM	1398	N	GLY	D	65	72.817	11.035	32.609	1.00	27.07
ATOM	1399	CA	GLY	D	65	73.882	11.019	33.616	1.00	26.85
ATOM	1400	C	GLY	D	65	75.190	11.651	33.183	1.00	30.69
ATOM	1401	O	GLY	D	65	76.089	11.825	33.997	1.00	31.19
ATOM	1402	N	SER	D	66	75.287	12.036	31.912	1.00	25.88
ATOM	1403	CA	SER	D	66	76.495	12.662	31.399	1.00	24.31
ATOM	1404	C	SER	D	66	76.682	14.113	31.883	1.00	28.10
ATOM	1405	O	SER	D	66	77.793	14.654	31.888	1.00	29.06
ATOM	1406	CB	SER	D	66	76.454	12.648	29.857	1.00	25.33
ATOM	1407	OG	SER	D	66	75.428	13.550	29.364	1.00	25.27
ATOM	1408	N	ARG	D	67	75.564	14.771	32.247	1.00	21.92
ATOM	1409	CA	ARG	D	67	75.571	16.157	32.680	1.00	20.64
ATOM	1410	C	ARG	D	67	76.060	17.130	31.581	1.00	21.33
ATOM	1411	O	ARG	D	67	76.476	18.236	31.854	1.00	23.88
ATOM	1412	CB	ARG	D	67	76.274	16.320	34.033	1.00	24.90
ATOM	1413	CG	ARG	D	67	75.630	15.331	35.037	1.00	34.18
ATOM	1414	CD	ARG	D	67	75.927	15.626	36.478	1.00	41.97
ATOM	1415	NE	ARG	D	67	77.213	15.050	36.869	1.00	42.73
ATOM	1416	CZ	ARG	D	67	77.511	13.750	37.086	1.00	50.11
ATOM	1417	NH1	ARG	D	67	76.638	12.732	36.977	1.00	32.87
ATOM	1418	NH2	ARG	D	67	78.761	13.476	37.438	1.00	35.89
ATOM	1419	N	ILE	D	68	75.922	16.675	30.337	1.00	20.99
ATOM	1420	CA	ILE	D	68	76.342	17.482	29.196	1.00	19.82

ATOM	1421	C	ILE	D	68	75.308	18.552	28.761	1.00	18.74
ATOM	1422	O	ILE	D	68	74.063	18.354	28.842	1.00	18.59
ATOM	1423	CB	ILE	D	68	76.553	16.552	27.943	1.00	22.72
ATOM	1424	CG1	ILE	D	68	77.870	15.741	28.011	1.00	22.79
ATOM	1425	CG2	ILE	D	68	76.492	17.349	26.604	1.00	23.66
ATOM	1426	CD1	ILE	D	68	77.831	14.542	27.090	1.00	24.22
ATOM	1427	N	ILE	D	69	75.866	19.651	28.331	1.00	17.03
ATOM	1428	CA	ILE	D	69	75.133	20.812	27.729	1.00	16.07
ATOM	1429	C	ILE	D	69	76.113	21.177	26.568	1.00	18.47
ATOM	1430	O	ILE	D	69	77.135	21.853	26.785	1.00	19.41
ATOM	1431	CB	ILE	D	69	74.990	22.034	28.619	1.00	17.97
ATOM	1432	CG1	ILE	D	69	74.094	21.722	29.861	1.00	17.84
ATOM	1433	CG2	ILE	D	69	74.318	23.224	27.796	1.00	14.87
ATOM	1434	CD1	ILE	D	69	72.656	21.278	29.519	1.00	16.76
ATOM	1435	N	SER	D	70	75.800	20.705	25.359	1.00	16.82
ATOM	1436	CA	SER	D	70	76.694	20.960	24.186	1.00	16.67
ATOM	1437	C	SER	D	70	76.030	21.879	23.159	1.00	16.91
ATOM	1438	O	SER	D	70	74.926	21.572	22.658	1.00	17.58
ATOM	1439	CB	SER	D	70	77.011	19.630	23.537	1.00	19.85
ATOM	1440	OG	SER	D	70	77.957	19.775	22.482	1.00	22.39
ATOM	1441	N	VAL	D	71	76.695	22.980	22.865	1.00	16.01
ATOM	1442	CA	VAL	D	71	76.145	23.963	21.853	1.00	17.80
ATOM	1443	C	VAL	D	71	76.803	23.589	20.516	1.00	22.32
ATOM	1444	O	VAL	D	71	78.012	23.676	20.369	1.00	23.49
ATOM	1445	CB	VAL	D	71	76.329	25.399	22.263	1.00	22.83
ATOM	1446	CG1	VAL	D	71	75.507	25.648	23.572	1.00	21.98
ATOM	1447	CG2	VAL	D	71	77.809	25.768	22.399	1.00	24.06
ATOM	1448	N	ASN	D	72	75.970	23.121	19.584	1.00	20.48
ATOM	1449	CA	ASN	D	72	76.427	22.621	18.267	1.00	20.13
ATOM	1450	C	ASN	D	72	75.998	23.462	17.099	1.00	22.39
ATOM	1451	O	ASN	D	72	75.023	24.219	17.165	1.00	22.18
ATOM	1452	CB	ASN	D	72	75.811	21.233	18.033	1.00	21.77
ATOM	1453	CG	ASN	D	72	76.097	20.254	19.165	1.00	30.59
ATOM	1454	OD1	ASN	D	72	77.069	20.428	19.917	1.00	25.69
ATOM	1455	ND2	ASN	D	72	75.228	19.241	19.317	1.00	26.90
ATOM	1456	N	GLY	D	73	76.708	23.283	15.994	1.00	20.53
ATOM	1457	CA	GLY	D	73	76.343	24.046	14.794	1.00	19.66
ATOM	1458	C	GLY	D	73	76.636	25.528	14.994	1.00	20.18
ATOM	1459	O	GLY	D	73	77.584	25.917	15.706	1.00	19.03
ATOM	1460	N	ALA	D	74	75.821	26.380	14.343	1.00	16.73
ATOM	1461	CA	ALA	D	74	76.006	27.831	14.434	1.00	16.27
ATOM	1462	C	ALA	D	74	75.988	28.387	15.874	1.00	17.37
ATOM	1463	O	ALA	D	74	76.616	29.406	16.149	1.00	18.06
ATOM	1464	CB	ALA	D	74	74.987	28.616	13.530	1.00	17.59
ATOM	1465	N	ALA	D	75	75.226	27.686	16.729	1.00	17.95
ATOM	1466	CA	ALA	D	75	75.069	28.102	18.147	1.00	17.42
ATOM	1467	C	ALA	D	75	76.415	28.126	18.870	1.00	19.91
ATOM	1468	O	ALA	D	75	76.543	28.800	19.897	1.00	19.81
ATOM	1469	CB	ALA	D	75	74.115	27.217	18.827	1.00	18.30
ATOM	1470	N	ALA	D	76	77.433	27.422	18.345	1.00	16.78
ATOM	1471	CA	ALA	D	76	78.747	27.455	18.982	1.00	18.31
ATOM	1472	C	ALA	D	76	79.347	28.882	18.991	1.00	18.92
ATOM	1473	O	ALA	D	76	80.266	29.184	19.740	1.00	19.50
ATOM	1474	CB	ALA	D	76	79.684	26.446	18.309	1.00	19.95
ATOM	1475	N	HIS	D	77	78.830	29.800	18.149	1.00	16.41
ATOM	1476	CA	HIS	D	77	79.302	31.149	18.115	1.00	17.43
ATOM	1477	C	HIS	D	77	78.710	32.014	19.243	1.00	18.10
ATOM	1478	O	HIS	D	77	79.143	33.147	19.435	1.00	20.06
ATOM	1479	CB	HIS	D	77	78.785	31.847	16.791	1.00	19.37
ATOM	1480	CG	HIS	D	77	79.540	31.470	15.545	1.00	22.65

ATOM	1481	ND1	HIS	D	77	80.667	32.145	15.137	1.00	25.27
ATOM	1482	CD2	HIS	D	77	79.308	30.523	14.605	1.00	22.98
ATOM	1483	CE1	HIS	D	77	81.109	31.624	14.002	1.00	24.52
ATOM	1484	NE2	HIS	D	77	80.307	30.637	13.657	1.00	23.17
ATOM	1485	N	CYS	D	78	77.694	31.475	19.940	1.00	17.70
ATOM	1486	CA	CYS	D	78	76.964	32.234	20.974	1.00	18.05
ATOM	1487	C	CYS	D	78	77.251	31.832	22.400	1.00	21.51
ATOM	1488	O	CYS	D	78	76.750	32.470	23.321	1.00	21.14
ATOM	1489	CB	CYS	D	78	75.466	32.047	20.753	1.00	19.61
ATOM	1490	SG	CYS	D	78	74.878	32.588	19.098	1.00	25.07
ATOM	1491	N	ALA	D	79	78.033	30.778	22.586	1.00	20.09
ATOM	1492	CA	ALA	D	79	78.365	30.353	23.943	1.00	19.73
ATOM	1493	C	ALA	D	79	79.677	29.603	23.922	1.00	25.47
ATOM	1494	O	ALA	D	79	80.013	28.966	22.934	1.00	23.97
ATOM	1495	CB	ALA	D	79	77.283	29.479	24.512	1.00	20.06
ATOM	1496	N	SER	D	80	80.406	29.664	25.036	1.00	21.56
ATOM	1497	CA	SER	D	80	81.697	28.965	25.191	1.00	22.17
ATOM	1498	C	SER	D	80	81.623	28.023	26.379	1.00	23.37
ATOM	1499	O	SER	D	80	80.792	28.213	27.275	1.00	21.62
ATOM	1500	CB	SER	D	80	82.824	29.931	25.485	1.00	25.03
ATOM	1501	OG	SER	D	80	82.930	30.986	24.543	1.00	28.26
ATOM	1502	N	VAL	D	81	82.499	27.021	26.388	1.00	18.88
ATOM	1503	CA	VAL	D	81	82.548	26.053	27.491	1.00	19.13
ATOM	1504	C	VAL	D	81	82.739	26.876	28.769	1.00	21.75
ATOM	1505	O	VAL	D	81	83.558	27.824	28.819	1.00	20.90
ATOM	1506	CB	VAL	D	81	83.722	25.072	27.272	1.00	21.73
ATOM	1507	CG1	VAL	D	81	83.986	24.271	28.562	1.00	22.57
ATOM	1508	CG2	VAL	D	81	83.366	24.099	26.155	1.00	21.80
ATOM	1509	N	GLY	D	82	81.973	26.526	29.798	1.00	18.71
ATOM	1510	CA	GLY	D	82	82.060	27.276	31.055	1.00	18.70
ATOM	1511	C	GLY	D	82	81.007	28.365	31.234	1.00	22.87
ATOM	1512	O	GLY	D	82	80.782	28.830	32.338	1.00	22.78
ATOM	1513	N	ASP	D	83	80.366	28.835	30.145	1.00	16.66
ATOM	1514	CA	ASP	D	83	79.356	29.867	30.305	1.00	16.76
ATOM	1515	C	ASP	D	83	78.131	29.322	31.070	1.00	16.77
ATOM	1516	O	ASP	D	83	77.748	28.153	30.896	1.00	17.18
ATOM	1517	CB	ASP	D	83	78.861	30.294	28.908	1.00	18.79
ATOM	1518	CG	ASP	D	83	79.852	31.196	28.164	1.00	22.59
ATOM	1519	OD1	ASP	D	83	80.935	31.544	28.680	1.00	20.93
ATOM	1520	OD2	ASP	D	83	79.519	31.615	27.015	1.00	21.88
ATOM	1521	N	ILE	D	84	77.515	30.198	31.860	1.00	17.58
ATOM	1522	CA	ILE	D	84	76.300	29.822	32.603	1.00	17.77
ATOM	1523	C	ILE	D	84	75.119	30.302	31.751	1.00	17.52
ATOM	1524	O	ILE	D	84	75.119	31.474	31.351	1.00	16.51
ATOM	1525	CB	ILE	D	84	76.296	30.573	33.935	1.00	21.87
ATOM	1526	CG1	ILE	D	84	77.513	30.116	34.766	1.00	22.20
ATOM	1527	CG2	ILE	D	84	74.978	30.346	34.726	1.00	22.70
ATOM	1528	CD1	ILE	D	84	77.676	31.008	36.011	1.00	27.68
ATOM	1529	N	VAL	D	85	74.192	29.388	31.497	1.00	16.68
ATOM	1530	CA	VAL	D	85	73.007	29.731	30.686	1.00	14.93
ATOM	1531	C	VAL	D	85	71.700	29.265	31.326	1.00	18.77
ATOM	1532	O	VAL	D	85	71.702	28.445	32.264	1.00	18.51
ATOM	1533	CB	VAL	D	85	73.144	29.098	29.266	1.00	15.49
ATOM	1534	CG1	VAL	D	85	74.452	29.475	28.627	1.00	16.44
ATOM	1535	CG2	VAL	D	85	73.026	27.645	29.306	1.00	14.40
ATOM	1536	N	ILE	D	86	70.571	29.792	30.807	1.00	14.77
ATOM	1537	CA	ILE	D	86	69.244	29.418	31.229	1.00	15.52
ATOM	1538	C	ILE	D	86	68.618	28.876	29.933	1.00	15.28
ATOM	1539	O	ILE	D	86	68.730	29.572	28.899	1.00	15.56
ATOM	1540	CB	ILE	D	86	68.442	30.582	31.786	1.00	18.22

ATOM	1541	CG1	ILE	D	86	69.034	31.030	33.158	1.00	19.52
ATOM	1542	CG2	ILE	D	86	66.998	30.177	31.976	1.00	18.36
ATOM	1543	CD1	ILE	D	86	68.686	32.448	33.495	1.00	25.25
ATOM	1544	N	ILE	D	87	68.087	27.692	29.954	1.00	11.80
ATOM	1545	CA	ILE	D	87	67.466	27.037	28.747	1.00	11.37
ATOM	1546	C	ILE	D	87	65.989	26.902	29.021	1.00	16.80
ATOM	1547	O	ILE	D	87	65.585	26.259	30.043	1.00	15.75
ATOM	1548	CB	ILE	D	87	68.096	25.681	28.476	1.00	14.04
ATOM	1549	CG1	ILE	D	87	69.636	25.844	28.325	1.00	14.68
ATOM	1550	CG2	ILE	D	87	67.438	24.977	27.201	1.00	16.46
ATOM	1551	CD1	ILE	D	87	70.419	24.558	27.961	1.00	16.93
ATOM	1552	N	ALA	D	88	65.127	27.457	28.161	1.00	13.54
ATOM	1553	CA	ALA	D	88	63.667	27.410	28.397	1.00	12.01
ATOM	1554	C	ALA	D	88	62.870	26.916	27.216	1.00	15.27
ATOM	1555	O	ALA	D	88	63.341	27.080	26.077	1.00	14.13
ATOM	1556	CB	ALA	D	88	63.197	28.842	28.683	1.00	12.68
ATOM	1557	N	SER	D	89	61.703	26.359	27.432	1.00	11.75
ATOM	1558	CA	SER	D	89	60.793	26.000	26.336	1.00	9.22
ATOM	1559	C	SER	D	89	59.463	26.672	26.691	1.00	13.85
ATOM	1560	O	SER	D	89	59.122	26.881	27.894	1.00	12.02
ATOM	1561	CB	SER	D	89	60.657	24.533	26.038	1.00	13.00
ATOM	1562	OG	SER	D	89	59.637	23.875	26.787	1.00	13.68
ATOM	1563	N	PHE	D	90	58.652	27.010	25.690	1.00	9.51
ATOM	1564	CA	PHE	D	90	57.352	27.650	25.837	1.00	10.69
ATOM	1565	C	PHE	D	90	56.272	26.831	25.169	1.00	14.12
ATOM	1566	O	PHE	D	90	56.519	26.218	24.124	1.00	13.43
ATOM	1567	CB	PHE	D	90	57.381	29.069	25.211	1.00	9.99
ATOM	1568	CG	PHE	D	90	58.172	30.051	26.052	1.00	8.63
ATOM	1569	CD1	PHE	D	90	59.569	30.106	25.972	1.00	12.75
ATOM	1570	CD2	PHE	D	90	57.492	30.917	26.943	1.00	9.84
ATOM	1571	CE1	PHE	D	90	60.296	31.033	26.745	1.00	12.66
ATOM	1572	CE2	PHE	D	90	58.223	31.786	27.752	1.00	11.34
ATOM	1573	CZ	PHE	D	90	59.576	31.884	27.669	1.00	11.79
ATOM	1574	N	VAL	D	91	55.074	26.811	25.733	1.00	11.04
ATOM	1575	CA	VAL	D	91	53.934	26.075	25.155	1.00	8.97
ATOM	1576	C	VAL	D	91	52.749	27.000	25.053	1.00	12.88
ATOM	1577	O	VAL	D	91	52.705	28.071	25.735	1.00	13.37
ATOM	1578	CB	VAL	D	91	53.519	24.811	25.939	1.00	11.62
ATOM	1579	CG1	VAL	D	91	54.527	23.721	25.805	1.00	11.91
ATOM	1580	CG2	VAL	D	91	53.294	25.194	27.489	1.00	13.43
ATOM	1581	N	THR	D	92	51.759	26.638	24.210	1.00	11.67
ATOM	1582	CA	THR	D	92	50.571	27.439	24.086	1.00	9.61
ATOM	1583	C	THR	D	92	49.326	26.678	24.633	1.00	8.31
ATOM	1584	O	THR	D	92	49.266	25.473	24.646	1.00	11.35
ATOM	1585	CB	THR	D	92	50.371	27.971	22.630	1.00	12.02
ATOM	1586	OG1	THR	D	92	50.296	26.819	21.738	1.00	17.42
ATOM	1587	CG2	THR	D	92	51.481	28.893	22.269	1.00	11.07
ATOM	1588	N	MET	D	93	48.330	27.441	25.059	1.00	10.31
ATOM	1589	CA	MET	D	93	47.103	26.859	25.667	1.00	10.55
ATOM	1590	C	MET	D	93	46.090	27.986	25.846	1.00	10.55
ATOM	1591	O	MET	D	93	46.444	29.174	25.900	1.00	11.69
ATOM	1592	CB	MET	D	93	47.421	26.236	27.109	1.00	11.27
ATOM	1593	CG	MET	D	93	47.856	27.339	28.054	1.00	11.07
ATOM	1594	SD	MET	D	93	48.572	26.650	29.641	1.00	13.35
ATOM	1595	CE	MET	D	93	50.133	26.102	28.965	1.00	13.30
ATOM	1596	N	PRO	D	94	44.820	27.596	25.967	1.00	10.89
ATOM	1597	CA	PRO	D	94	43.757	28.594	26.172	1.00	10.92
ATOM	1598	C	PRO	D	94	43.959	29.439	27.445	1.00	13.89
ATOM	1599	O	PRO	D	94	44.529	28.930	28.444	1.00	13.64
ATOM	1600	CB	PRO	D	94	42.492	27.750	26.291	1.00	15.15

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ATOM   1601  CG  PRO D  94      42.839  26.445  25.629  1.00 18.73
ATOM   1602  CD  PRO D  94      44.315  26.240  25.823  1.00 13.59
ATOM   1603  N   ASP D  95      43.535  30.684  27.413  1.00 12.77
ATOM   1604  CA  ASP D  95      43.665  31.614  28.524  1.00 11.85
ATOM   1605  C   ASP D  95      43.174  30.951  29.847  1.00 12.73
ATOM   1606  O   ASP D  95      43.865  31.103  30.918  1.00 14.23
ATOM   1607  CB  ASP D  95      42.811  32.862  28.257  1.00 13.88
ATOM   1608  CG  ASP D  95      42.966  33.903  29.322  1.00 16.93
ATOM   1609  OD1 ASP D  95      44.066  34.422  29.557  1.00 15.12
ATOM   1610  OD2 ASP D  95      41.944  34.159  30.004  1.00 25.27
ATOM   1611  N   GLU D  96      42.037  30.280  29.777  1.00 11.92
ATOM   1612  CA  GLU D  96      41.450  29.634  31.006  1.00 13.09
ATOM   1613  C   GLU D  96      42.418  28.668  31.670  1.00 17.50
ATOM   1614  O   GLU D  96      42.463  28.607  32.916  1.00 17.59
ATOM   1615  CB  GLU D  96      40.194  28.900  30.623  1.00 15.73
ATOM   1616  CG  GLU D  96      39.407  28.382  31.819  1.00 27.44
ATOM   1617  CD  GLU D  96      39.718  26.953  32.150  1.00 46.48
ATOM   1618  OE1 GLU D  96      40.247  26.230  31.298  1.00 32.53
ATOM   1619  OE2 GLU D  96      39.416  26.541  33.300  1.00 50.29
ATOM   1620  N   GLU D  97      43.184  27.904  30.898  1.00 13.12
ATOM   1621  CA  GLU D  97      44.151  26.962  31.475  1.00 11.58
ATOM   1622  C   GLU D  97      45.417  27.747  31.906  1.00 14.13
ATOM   1623  O   GLU D  97      46.124  27.431  32.874  1.00 14.05
ATOM   1624  CB  GLU D  97      44.553  25.876  30.429  1.00 10.79
ATOM   1625  CG  GLU D  97      43.463  24.971  30.050  1.00 12.84
ATOM   1626  CD  GLU D  97      43.862  23.894  29.037  1.00 16.10
ATOM   1627  OE1 GLU D  97      44.997  23.908  28.435  1.00 17.56
ATOM   1628  OE2 GLU D  97      43.042  22.981  28.897  1.00 19.58
ATOM   1629  N   ALA D  98      45.828  28.763  31.147  1.00 11.26
ATOM   1630  CA  ALA D  98      47.011  29.521  31.441  1.00 12.13
ATOM   1631  C   ALA D  98      47.025  30.209  32.830  1.00 12.78
ATOM   1632  O   ALA D  98      48.121  30.395  33.423  1.00 12.87
ATOM   1633  CB  ALA D  98      47.161  30.609  30.303  1.00 13.93
ATOM   1634  N   ARG D  99      45.795  30.577  33.268  1.00 13.12
ATOM   1635  CA  ARG D  99      45.668  31.263  34.534  1.00 13.91
ATOM   1636  C   ARG D  99      46.164  30.394  35.692  1.00 15.52
ATOM   1637  O   ARG D  99      46.555  30.998  36.715  1.00 16.74
ATOM   1638  CB  ARG D  99      44.232  31.694  34.717  1.00 13.81
ATOM   1639  CG  ARG D  99      43.930  32.832  33.737  1.00 21.54
ATOM   1640  CD  ARG D  99      42.544  33.302  33.768  1.00 31.31
ATOM   1641  NE  ARG D  99      42.382  34.329  32.737  1.00 34.14
ATOM   1642  CZ  ARG D  99      42.824  35.587  32.820  1.00 39.78
ATOM   1643  NH1 ARG D  99      43.448  36.028  33.912  1.00 39.29
ATOM   1644  NH2 ARG D  99      42.622  36.428  31.821  1.00 34.68
ATOM   1645  N   THR D 100      46.189  29.072  35.553  1.00 12.99
ATOM   1646  CA  THR D 100      46.668  28.209  36.674  1.00 13.08
ATOM   1647  C   THR D 100      47.916  27.391  36.307  1.00 15.62
ATOM   1648  O   THR D 100      48.408  26.541  37.068  1.00 16.66
ATOM   1649  CB  THR D 100      45.537  27.276  37.099  1.00 15.79
ATOM   1650  OG1 THR D 100      45.017  26.550  35.988  1.00 14.58
ATOM   1651  CG2 THR D 100      44.344  28.091  37.708  1.00 15.05
ATOM   1652  N   TRP D 101      48.490  27.635  35.105  1.00 14.25
ATOM   1653  CA  TRP D 101      49.645  26.857  34.699  1.00 13.12
ATOM   1654  C   TRP D 101      50.846  27.042  35.554  1.00 15.17
ATOM   1655  O   TRP D 101      51.111  28.163  36.042  1.00 16.82
ATOM   1656  CB  TRP D 101      49.970  27.286  33.191  1.00 11.79
ATOM   1657  CG  TRP D 101      51.197  26.624  32.676  1.00 10.50
ATOM   1658  CD1 TRP D 101      52.416  27.164  32.527  1.00 12.40
ATOM   1659  CD2 TRP D 101      51.317  25.240  32.383  1.00 12.89
ATOM   1660  NE1 TRP D 101      53.292  26.208  32.121  1.00 12.65
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ATOM   1661  CE2 TRP D 101      52.659  25.019  32.000  1.00 13.88
ATOM   1662  CE3 TRP D 101      50.419  24.168  32.362  1.00 15.74
ATOM   1663  CZ2 TRP D 101      53.144  23.769  31.624  1.00 16.20
ATOM   1664  CZ3 TRP D 101      50.898  22.888  32.009  1.00 19.25
ATOM   1665  CH2 TRP D 101      52.266  22.699  31.649  1.00 19.62
ATOM   1666  N   ARG D 102      51.613  25.952  35.714  1.00 15.08
ATOM   1667  CA  ARG D 102      52.844  25.993  36.481  1.00 15.90
ATOM   1668  C   ARG D 102      53.983  25.375  35.637  1.00 11.33
ATOM   1669  O   ARG D 102      53.846  24.253  35.202  1.00 14.41
ATOM   1670  CB  ARG D 102      52.703  25.128  37.779  1.00 18.89
ATOM   1671  CG  ARG D 102      51.612  25.639  38.780  1.00 24.40
ATOM   1672  CD  ARG D 102      51.559  24.821  40.096  1.00 22.77
ATOM   1673  NE  ARG D 102      52.794  24.906  40.846  1.00 27.18
ATOM   1674  CZ  ARG D 102      53.120  25.887  41.689  1.00 28.35
ATOM   1675  NH1 ARG D 102      52.313  26.911  41.893  1.00 23.60
ATOM   1676  NH2 ARG D 102      54.280  25.844  42.314  1.00 31.92
ATOM   1677  N   PRO D 103      55.088  26.106  35.497  1.00 12.26
ATOM   1678  CA  PRO D 103      56.234  25.566  34.721  1.00 13.54
ATOM   1679  C   PRO D 103      57.047  24.562  35.500  1.00 17.32
ATOM   1680  O   PRO D 103      56.956  24.539  36.792  1.00 16.83
ATOM   1681  CB  PRO D 103      57.114  26.794  34.506  1.00 14.38
ATOM   1682  CG  PRO D 103      56.894  27.640  35.767  1.00 22.25
ATOM   1683  CD  PRO D 103      55.363  27.456  36.011  1.00 16.38
ATOM   1684  N   ASN D 104      57.859  23.759  34.781  1.00 13.82
ATOM   1685  CA  ASN D 104      58.744  22.758  35.377  1.00 12.48
ATOM   1686  C   ASN D 104      60.121  23.389  35.504  1.00 19.52
ATOM   1687  O   ASN D 104      60.775  23.647  34.460  1.00 16.91
ATOM   1688  CB  ASN D 104      58.798  21.477  34.539  1.00 13.72
ATOM   1689  CG  ASN D 104      57.470  20.884  34.345  1.00 19.91
ATOM   1690  OD1 ASN D 104      56.775  20.587  35.338  1.00 17.05
ATOM   1691  ND2 ASN D 104      57.032  20.718  33.087  1.00 20.70
ATOM   1692  N   VAL D 105      60.613  23.649  36.722  1.00 17.67
ATOM   1693  CA  VAL D 105      61.885  24.295  36.850  1.00 16.36
ATOM   1694  C   VAL D 105      62.907  23.448  37.546  1.00 21.93
ATOM   1695  O   VAL D 105      62.601  22.863  38.602  1.00 22.45
ATOM   1696  CB  VAL D 105      61.775  25.635  37.634  1.00 18.76
ATOM   1697  CG1 VAL D 105      63.106  26.314  37.743  1.00 19.86
ATOM   1698  CG2 VAL D 105      60.642  26.573  37.039  1.00 19.00
ATOM   1699  N   ALA D 106      64.102  23.365  36.974  1.00 20.08
ATOM   1700  CA  ALA D 106      65.232  22.610  37.580  1.00 19.28
ATOM   1701  C   ALA D 106      66.330  23.614  37.866  1.00 22.54
ATOM   1702  O   ALA D 106      66.699  24.410  37.000  1.00 20.02
ATOM   1703  CB  ALA D 106      65.733  21.552  36.689  1.00 19.59
ATOM   1704  N   TYR D 107      66.894  23.609  39.098  1.00 21.77
ATOM   1705  CA  TYR D 107      67.952  24.556  39.469  1.00 22.90
ATOM   1706  C   TYR D 107      69.287  23.841  39.546  1.00 25.98
ATOM   1707  O   TYR D 107      69.335  22.668  39.882  1.00 25.22
ATOM   1708  CB  TYR D 107      67.646  25.222  40.818  1.00 25.00
ATOM   1709  CG  TYR D 107      66.482  26.167  40.752  1.00 24.25
ATOM   1710  CD1 TYR D 107      66.651  27.484  40.330  1.00 26.30
ATOM   1711  CD2 TYR D 107      65.202  25.733  41.102  1.00 25.93
ATOM   1712  CE1 TYR D 107      65.588  28.344  40.270  1.00 29.13
ATOM   1713  CE2 TYR D 107      64.125  26.600  41.056  1.00 25.26
ATOM   1714  CZ  TYR D 107      64.325  27.900  40.658  1.00 31.88
ATOM   1715  OH  TYR D 107      63.238  28.756  40.594  1.00 35.96
ATOM   1716  N   PHE D 108      70.356  24.556  39.194  1.00 26.53
ATOM   1717  CA  PHE D 108      71.677  23.953  39.185  1.00 25.71
ATOM   1718  C   PHE D 108      72.739  24.852  39.791  1.00 31.22
ATOM   1719  O   PHE D 108      72.611  26.079  39.860  1.00 28.62
ATOM   1720  CB  PHE D 108      72.145  23.669  37.719  1.00 25.29
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ATOM	1721	CG	PHE	D	108	71.302	22.678	36.974	1.00	21.78
ATOM	1722	CD1	PHE	D	108	70.101	23.072	36.357	1.00	19.05
ATOM	1723	CD2	PHE	D	108	71.708	21.360	36.850	1.00	20.20
ATOM	1724	CE1	PHE	D	108	69.333	22.156	35.675	1.00	19.07
ATOM	1725	CE2	PHE	D	108	70.965	20.441	36.163	1.00	22.77
ATOM	1726	CZ	PHE	D	108	69.733	20.879	35.546	1.00	20.24
ATOM	1727	N	GLU	D	109	73.815	24.196	40.198	1.00	30.97
ATOM	1728	CA	GLU	D	109	74.970	24.855	40.797	1.00	32.90
ATOM	1729	C	GLU	D	109	76.205	24.037	40.466	1.00	33.93
ATOM	1730	O	GLU	D	109	76.114	22.898	40.055	1.00	30.42
ATOM	1731	CB	GLU	D	109	74.826	24.827	42.326	1.00	35.17
ATOM	1732	CG	GLU	D	109	74.907	23.400	42.875	1.00	44.89
ATOM	1733	CD	GLU	D	109	74.607	23.314	44.352	1.00	68.70
ATOM	1734	OE1	GLU	D	109	74.608	24.376	45.020	1.00	58.38
ATOM	1735	OE2	GLU	D	109	74.358	22.182	44.842	1.00	66.11
ATOM	1736	N	GLY	D	110	77.379	24.614	40.702	1.00	33.06
ATOM	1737	CA	GLY	D	110	78.616	23.899	40.454	1.00	32.35
ATOM	1738	C	GLY	D	110	78.689	23.323	39.056	1.00	35.50
ATOM	1739	O	GLY	D	110	78.449	24.039	38.072	1.00	35.53
ATOM	1740	N	ASP	D	111	79.074	22.063	38.971	1.00	29.97
ATOM	1741	CA	ASP	D	111	79.232	21.400	37.693	1.00	31.05
ATOM	1742	C	ASP	D	111	77.960	20.672	37.285	1.00	30.82
ATOM	1743	O	ASP	D	111	77.886	19.418	37.225	1.00	28.67
ATOM	1744	CB	ASP	D	111	80.465	20.495	37.717	1.00	33.49
ATOM	1745	CG	ASP	D	111	80.534	19.558	36.541	1.00	44.31
ATOM	1746	OD1	ASP	D	111	80.219	19.999	35.400	1.00	46.12
ATOM	1747	OD2	ASP	D	111	80.882	18.378	36.760	1.00	41.60
ATOM	1748	N	ASN	D	112	76.959	21.480	36.967	1.00	27.75
ATOM	1749	CA	ASN	D	112	75.682	20.951	36.556	1.00	25.85
ATOM	1750	C	ASN	D	112	75.072	20.013	37.556	1.00	28.56
ATOM	1751	O	ASN	D	112	74.553	18.956	37.211	1.00	24.07
ATOM	1752	CB	ASN	D	112	75.744	20.367	35.149	1.00	25.14
ATOM	1753	CG	ASN	D	112	75.975	21.425	34.158	1.00	19.48
ATOM	1754	OD1	ASN	D	112	75.875	22.600	34.511	1.00	22.70
ATOM	1755	ND2	ASN	D	112	76.334	21.051	32.918	1.00	21.36
ATOM	1756	N	GLU	D	113	75.142	20.436	38.818	1.00	27.11
ATOM	1757	CA	GLU	D	113	74.556	19.639	39.900	1.00	28.84
ATOM	1758	C	GLU	D	113	73.181	20.182	40.147	1.00	27.72
ATOM	1759	O	GLU	D	113	73.039	21.365	40.555	1.00	26.82
ATOM	1760	CB	GLU	D	113	75.388	19.695	41.177	1.00	30.87
ATOM	1761	CG	GLU	D	113	76.724	18.975	41.092	1.00	37.93
ATOM	1762	CD	GLU	D	113	76.692	17.429	41.016	1.00	59.74
ATOM	1763	OE1	GLU	D	113	75.612	16.786	40.882	1.00	46.50
ATOM	1764	OE2	GLU	D	113	77.814	16.868	41.082	1.00	59.60
ATOM	1765	N	MET	D	114	72.194	19.333	39.866	1.00	27.25
ATOM	1766	CA	MET	D	114	70.781	19.680	40.012	1.00	32.32
ATOM	1767	C	MET	D	114	70.391	19.716	41.452	1.00	39.86
ATOM	1768	O	MET	D	114	70.527	18.703	42.145	1.00	40.94
ATOM	1769	CB	MET	D	114	69.889	18.646	39.319	1.00	34.33
ATOM	1770	CG	MET	D	114	68.468	19.136	39.198	1.00	36.77
ATOM	1771	SD	MET	D	114	67.314	17.889	38.726	1.00	39.76
ATOM	1772	CE	MET	D	114	67.664	17.803	36.803	1.00	31.31
ATOM	1773	N	LYS	D	115	69.893	20.851	41.915	1.00	37.37
ATOM	1774	CA	LYS	D	115	69.488	20.983	43.324	1.00	38.95
ATOM	1775	C	LYS	D	115	68.169	20.274	43.622	1.00	54.19
ATOM	1776	O	LYS	D	115	67.301	20.213	42.705	1.00	51.66
ATOM	1777	CB	LYS	D	115	69.362	22.437	43.715	1.00	41.43
ATOM	1778	CG	LYS	D	115	70.655	23.235	43.740	1.00	47.27
ATOM	1779	CD	LYS	D	115	70.334	24.681	44.041	1.00	43.78
ATOM	1780	CE	LYS	D	115	71.439	25.627	43.660	1.00	55.99

ATOM	1781	NZ	LYS	D	115	71.276	26.945	44.363	1.00	62.59
ATOM	1783	OW0	WAT	G	1	50.690	34.966	25.739	1.00	12.46
ATOM	1784	OW0	WAT	G	2	65.358	37.341	23.976	1.00	14.50
ATOM	1785	OW0	WAT	G	3	53.112	36.553	25.090	1.00	12.96
ATOM	1786	OW0	WAT	G	4	59.501	34.869	25.680	1.00	16.21
ATOM	1787	OW0	WAT	G	5	42.457	44.697	14.900	1.00	16.96
ATOM	1788	OW0	WAT	G	6	62.264	42.848	18.466	1.00	12.78
ATOM	1789	OW0	WAT	G	7	60.346	41.648	20.211	1.00	14.43
ATOM	1790	OW0	WAT	G	8	49.376	37.618	12.957	1.00	11.87
ATOM	1791	OW0	WAT	G	9	43.082	43.742	4.464	1.00	15.75
ATOM	1792	OW0	WAT	G	10	57.736	40.739	19.570	1.00	18.14
ATOM	1793	OW0	WAT	G	11	53.768	31.148	15.023	1.00	18.49
ATOM	1794	OW0	WAT	G	12	46.397	19.640	8.284	1.00	20.49
ATOM	1795	OW0	WAT	G	13	49.398	32.153	35.416	1.00	15.58
ATOM	1796	OW0	WAT	G	14	52.292	38.335	12.919	1.00	12.77
ATOM	1797	OW0	WAT	G	15	55.884	41.199	17.565	1.00	17.15
ATOM	1798	OW0	WAT	G	16	68.646	41.874	7.890	1.00	18.45
ATOM	1799	OW0	WAT	G	17	60.172	36.501	11.568	1.00	20.08
ATOM	1800	OW0	WAT	G	18	52.295	33.705	18.070	1.00	19.24
ATOM	1801	OW0	WAT	G	19	43.878	46.628	8.547	1.00	18.83
ATOM	1802	OW0	WAT	G	20	44.503	23.424	0.796	1.00	17.45
ATOM	1803	OW0	WAT	G	21	64.440	48.899	19.979	1.00	18.93
ATOM	1804	OW0	WAT	G	22	71.193	48.088	36.959	1.00	16.89
ATOM	1805	OW0	WAT	G	23	49.349	33.334	14.599	1.00	20.32
ATOM	1806	OW0	WAT	G	24	71.024	49.740	30.410	1.00	19.88
ATOM	1807	OW0	WAT	G	25	42.979	46.992	11.153	1.00	17.12
ATOM	1808	OW0	WAT	G	26	38.559	42.979	23.184	1.00	21.81
ATOM	1809	OW0	WAT	G	27	53.263	26.900	13.822	1.00	15.81
ATOM	1810	OW0	WAT	G	28	71.768	47.157	29.190	1.00	21.31
ATOM	1811	OW0	WAT	G	29	50.910	52.836	39.909	1.00	21.20
ATOM	1812	OW0	WAT	G	30	51.612	34.739	20.749	1.00	21.50
ATOM	1813	OW0	WAT	G	31	47.760	55.722	0.508	1.00	26.79
ATOM	1814	OW0	WAT	G	32	57.250	54.959	34.792	1.00	18.33
ATOM	1815	OW0	WAT	G	33	65.008	51.887	42.170	1.00	21.45
ATOM	1816	OW0	WAT	G	34	71.716	46.104	34.998	1.00	19.77
ATOM	1817	OW0	WAT	G	35	56.789	36.428	13.221	1.00	19.13
ATOM	1818	OW0	WAT	G	36	69.004	52.586	13.271	1.00	25.88
ATOM	1819	OW0	WAT	G	37	36.912	40.900	19.049	1.00	24.35
ATOM	1820	OW0	WAT	G	38	37.939	34.172	11.858	1.00	21.53
ATOM	1821	OW0	WAT	G	39	50.673	48.829	42.462	1.00	17.05
ATOM	1822	OW0	WAT	G	40	40.211	49.838	5.952	1.00	26.29
ATOM	1823	OW0	WAT	G	41	46.904	53.941	31.892	1.00	26.19
ATOM	1824	OW0	WAT	G	42	69.397	54.598	32.144	1.00	21.59
ATOM	1825	OW0	WAT	G	43	42.745	49.698	11.329	1.00	28.13
ATOM	1826	OW0	WAT	G	44	69.038	43.121	14.087	1.00	27.79
ATOM	1827	OW0	WAT	G	45	37.919	36.710	9.225	1.00	22.42
ATOM	1828	OW0	WAT	G	46	62.878	47.097	42.928	1.00	24.58
ATOM	1829	OW0	WAT	G	47	39.794	32.943	21.142	1.00	24.59
ATOM	1830	OW0	WAT	G	48	45.700	54.348	15.115	1.00	34.46
ATOM	1831	OW0	WAT	G	49	59.403	48.140	46.193	1.00	20.52
ATOM	1832	OW0	WAT	G	50	60.684	31.160	37.777	1.00	29.82
ATOM	1833	OW0	WAT	G	51	49.475	50.666	40.460	1.00	22.18
ATOM	1834	OW0	WAT	G	52	39.653	24.604	5.289	1.00	17.35
ATOM	1835	OW0	WAT	G	53	59.252	56.969	34.916	1.00	19.50
ATOM	1836	OW0	WAT	G	54	69.096	53.771	10.568	1.00	27.87
ATOM	1837	OW0	WAT	G	55	66.440	38.568	14.149	1.00	30.16
ATOM	1838	OW0	WAT	G	56	65.406	57.383	14.154	1.00	26.01
ATOM	1839	OW0	WAT	G	57	41.137	23.132	3.518	1.00	23.54
ATOM	1840	OW0	WAT	G	58	49.156	50.953	21.456	1.00	30.99
ATOM	1841	OW0	WAT	G	59	57.860	36.323	24.017	1.00	20.83

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ATOM   1842  OW0 WAT G  60      57.496  33.962  11.899  1.00 21.39
ATOM   1843  OW0 WAT G  61      66.579  48.294  43.413  1.00 24.77
ATOM   1844  OW0 WAT G  62      54.871  38.598  18.657  1.00 25.45
ATOM   1845  OW0 WAT G  63      50.967  51.195  43.999  1.00 22.75
ATOM   1846  OW0 WAT G  64      44.140  29.593   6.643  1.00 21.96
ATOM   1847  OW0 WAT G  65      43.548  39.803  29.673  1.00 26.57
ATOM   1848  OW0 WAT G  66      36.492  44.150  10.666  1.00 24.57
ATOM   1849  OW0 WAT G  67      72.566  46.343  31.771  1.00 22.95
ATOM   1850  OW0 WAT G  68      48.293  59.724  10.894  1.00 26.76
ATOM   1851  OW0 WAT G  69      62.460  39.930  21.422  1.00 26.61
ATOM   1852  OW0 WAT G  70      56.208  39.397  15.274  1.00 20.01
ATOM   1853  OW0 WAT G  71      72.875  42.561  38.908  1.00 36.97
ATOM   1854  OW0 WAT G  72      68.365  44.087  20.849  1.00 29.26
ATOM   1855  OW0 WAT G  73      43.058  49.160  23.577  1.00 29.45
ATOM   1856  OW0 WAT G  74      70.366  27.891  40.490  1.00 33.14
ATOM   1857  OW0 WAT G  75      37.060  33.614  18.493  1.00 25.03
ATOM   1858  OW0 WAT G  76      43.652  50.031  19.379  1.00 36.34
ATOM   1859  OW0 WAT G  77      70.513  54.847   7.916  1.00 33.66
ATOM   1860  OW0 WAT G  78      74.648  42.946  34.418  1.00 46.06
ATOM   1861  OW0 WAT G  79      44.747  49.850  -0.304  1.00 26.95
ATOM   1862  OW0 WAT G  80      40.824  41.298  27.887  1.00 25.17
ATOM   1863  OW0 WAT G  81      41.107  45.630  12.507  1.00 25.41
ATOM   1864  OW0 WAT G  82      57.806  41.126  45.667  1.00 28.19
ATOM   1865  OW0 WAT G  83      51.183  54.617  -2.727  1.00 32.75
ATOM   1866  OW0 WAT G  84      43.186  49.347  27.882  1.00 28.33
ATOM   1867  OW0 WAT G  85      61.540  49.575  -4.582  1.00 35.95
ATOM   1868  OW0 WAT G  86      50.267  17.542   8.910  1.00 30.16
ATOM   1869  OW0 WAT G  87      36.217  32.811  13.941  1.00 28.34
ATOM   1870  OW0 WAT G  88      72.058  52.836  10.622  1.00 45.57
ATOM   1871  OW0 WAT G  89      61.348  58.887   3.805  1.00 30.95
ATOM   1872  OW0 WAT G  90      48.622  56.983  14.003  1.00 31.75
ATOM   1873  OW0 WAT G  91      51.936  33.480  13.709  1.00 26.64
ATOM   1874  OW0 WAT G  92      51.875  46.258  -5.376  1.00 34.61
ATOM   1875  OW0 WAT G  93      42.359  53.407  10.255  1.00 30.41
ATOM   1876  OW0 WAT G  94      52.890  57.749  15.136  1.00 30.22
ATOM   1877  OW0 WAT G  95      58.430  56.302  24.467  1.00 26.47
ATOM   1878  OW0 WAT G  96      37.197  41.147  21.811  1.00 24.52
ATOM   1879  OW0 WAT G  97      52.686  23.652  -1.094  1.00 25.58
ATOM   1880  OW0 WAT G  98      43.317  41.529  34.451  1.00 35.83
ATOM   1881  OW0 WAT G  99      50.916  40.421  46.697  1.00 31.62
ATOM   1882  OW0 WAT G 100      59.444  53.045  -1.297  1.00 35.13
ATOM   1883  OW0 WAT G 101      54.344  37.059  14.071  1.00 25.37
ATOM   1884  OW0 WAT G 102      39.161  35.171  23.645  1.00 22.49
ATOM   1885  OW0 WAT G 103      48.196  28.696  16.212  1.00 22.74
ATOM   1886  OW0 WAT G 104      51.803  31.025  19.010  1.00 23.17
ATOM   1887  OW0 WAT G 105      50.671  37.681  42.927  1.00 29.64
ATOM   1888  OW0 WAT G 106      62.180  51.664  -1.624  1.00 34.04
ATOM   1889  OW0 WAT G 107      52.524  59.538  42.266  1.00 35.09
ATOM   1890  OW0 WAT G 108      46.932  49.006  21.391  1.00 25.94
ATOM   1891  OW0 WAT G 109      37.499  38.570  22.800  1.00 26.50
ATOM   1892  OW0 WAT G 110      72.898  50.305  27.829  1.00 30.56
ATOM   1893  OW0 WAT G 111      67.993  56.760   5.901  1.00 29.70
ATOM   1894  OW0 WAT G 112      48.644  53.571  -1.398  1.00 35.84
ATOM   1895  OW0 WAT G 113      58.963  38.275  42.967  1.00 30.25
ATOM   1896  OW0 WAT G 114      48.644  29.728  18.792  1.00 30.45
ATOM   1897  OW0 WAT G 115      42.373  28.434   9.504  1.00 30.65
ATOM   1898  OW0 WAT G 116      48.337  17.998   4.927  1.00 26.85
ATOM   1899  OW0 WAT G 117      43.367  57.024   0.108  1.00 36.26
ATOM   1900  OW0 WAT G 118      55.991  35.183  42.088  1.00 33.36
ATOM   1901  OW0 WAT G 119      55.166  18.825   3.751  1.00 39.06
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ATOM	1902	OW0	WAT	G	120	36.538	34.658	16.002	1.00	23.39
ATOM	1903	OW0	WAT	G	121	38.971	45.277	10.960	1.00	32.00
ATOM	1904	OW0	WAT	G	122	45.394	39.705	40.673	1.00	28.95
ATOM	1905	OW0	WAT	G	123	64.660	56.850	28.096	1.00	31.43
ATOM	1906	OW0	WAT	G	124	31.495	39.706	12.940	1.00	30.11
ATOM	1907	OW0	WAT	G	125	66.898	41.660	19.788	1.00	37.52
ATOM	1908	OW0	WAT	G	126	59.279	62.353	6.022	1.00	30.85
ATOM	1909	OW0	WAT	G	127	54.862	34.329	17.654	1.00	28.43
ATOM	1910	OW0	WAT	G	128	46.944	36.876	-2.147	1.00	28.17
ATOM	1911	OW0	WAT	G	129	47.374	18.007	2.535	1.00	36.60
ATOM	1912	OW0	WAT	G	130	44.808	50.361	22.031	1.00	29.95
ATOM	1913	OW0	WAT	G	131	56.071	58.293	30.768	1.00	29.87
ATOM	1914	OW0	WAT	G	132	39.948	33.299	8.889	1.00	43.00
ATOM	1917	OW0	WAT	G	135	62.136	38.451	12.117	1.00	15.27
ATOM	1918	OW0	WAT	G	136	57.446	61.036	34.612	1.00	23.04
ATOM	1919	OW0	WAT	G	137	55.835	37.709	21.070	1.00	20.63
ATOM	1920	OW0	WAT	G	138	62.428	40.009	14.530	1.00	34.20
ATOM	1921	OW0	WAT	G	139	62.638	59.963	30.173	1.00	31.10
ATOM	1922	OW0	WAT	G	140	55.220	36.878	16.564	1.00	26.78
ATOM	1923	OW0	WAT	G	141	53.791	35.442	22.528	1.00	28.89
ATOM	1924	OW0	WAT	G	142	64.950	39.916	20.459	1.00	30.25
ATOM	1925	OW0	WAT	G	143	60.864	56.504	38.809	1.00	27.10
ATOM	1926	OW0	WAT	G	144	50.834	36.062	-3.236	1.00	24.20
ATOM	1927	OW0	WAT	G	145	57.988	31.870	13.658	1.00	27.16
ATOM	1928	OW0	WAT	G	146	59.420	50.371	43.012	1.00	27.11
ATOM	1929	OW0	WAT	G	147	41.507	31.122	20.116	1.00	27.47
ATOM	1930	OW0	WAT	G	148	60.586	52.675	43.032	1.00	29.71
ATOM	1931	OW0	WAT	G	149	46.395	26.704	16.386	1.00	36.67
ATOM	1932	OW0	WAT	G	150	65.273	33.456	33.695	1.00	30.16
ATOM	1933	OW0	WAT	G	151	64.591	41.448	18.391	1.00	28.63
ATOM	1934	OW0	WAT	G	152	48.864	29.166	-5.087	1.00	26.64
ATOM	1935	OW0	WAT	G	153	62.622	58.231	27.208	1.00	34.13
ATOM	1936	OW0	WAT	G	154	61.506	38.693	18.376	1.00	48.10
ATOM	1937	OW0	WAT	G	155	56.258	32.027	15.818	1.00	40.67
ATOM	1938	OW0	WAT	G	156	58.824	38.296	18.235	1.00	34.94
ATOM	1939	OW0	WAT	G	157	53.978	29.606	39.376	1.00	38.68
ATOM	1940	OW0	WAT	G	158	53.182	56.416	29.461	1.00	25.79
ATOM	1941	OW0	WAT	G	159	49.085	39.844	-3.201	1.00	29.14
ATOM	1942	OW0	WAT	G	160	60.344	34.232	21.770	1.00	38.25
ATOM	1943	OW0	WAT	G	161	51.797	60.535	-5.207	1.00	32.32
ATOM	1944	OW0	WAT	G	162	48.186	38.211	36.506	1.00	28.29
ATOM	1945	OW0	WAT	G	163	58.462	37.470	15.660	1.00	45.25
ATOM	1946	OW0	WAT	G	164	45.851	29.690	18.302	1.00	28.59
ATOM	1947	OW0	WAT	G	165	64.873	40.315	16.036	1.00	36.40
ATOM	1948	OW0	WAT	G	166	59.897	58.114	1.470	1.00	36.57
ATOM	1949	OW0	WAT	G	167	55.910	60.828	8.749	1.00	35.99
ATOM	1950	OW0	WAT	G	168	58.826	36.800	21.280	1.00	46.77
ATOM	1951	OW0	WAT	G	169	73.241	44.114	36.191	1.00	28.55
ATOM	1952	OW0	WAT	G	170	62.716	53.030	41.277	1.00	28.32
ATOM	1953	OW0	WAT	G	171	71.215	34.038	37.383	1.00	27.69
ATOM	1954	OW0	WAT	G	172	62.192	37.635	14.596	1.00	50.53
ATOM	1955	OW0	WAT	G	173	65.616	56.974	1.251	1.00	31.26
ATOM	1956	OW0	WAT	G	174	76.080	34.843	37.370	1.00	35.85
ATOM	1957	OW0	WAT	G	175	73.299	43.407	25.575	1.00	36.58
ATOM	1958	OW0	WAT	G	176	65.884	43.263	17.413	1.00	40.37
ATOM	1959	OW0	WAT	G	177	67.452	40.654	15.215	1.00	42.76
ATOM	1960	OW0	WAT	G	178	54.648	62.290	32.413	1.00	53.70
ATOM	1961	OW0	WAT	G	179	51.497	49.736	48.977	1.00	29.11
ATOM	1962	OW0	WAT	G	180	44.613	37.553	5.661	1.00	33.03
ATOM	1963	OW0	WAT	G	181	70.015	49.056	17.242	1.00	35.32

ATOM	1964	OW0	WAT	G	182	67.847	54.823	14.616	1.00 27.00
ATOM	1965	OW0	WAT	G	183	75.622	47.339	26.201	1.00 39.70
ATOM	1966	OW0	WAT	G	184	58.156	30.750	37.764	1.00 43.06
ATOM	1967	OW0	WAT	G	185	63.117	44.122	43.660	1.00 32.67
ATOM	1968	OW0	WAT	G	186	70.428	46.037	20.380	1.00 37.29
ATOM	1969	OW0	WAT	G	187	65.215	59.373	12.091	1.00 28.47
ATOM	1970	OW0	WAT	G	188	67.748	44.609	18.032	1.00 53.73
ATOM	1971	OW0	WAT	G	189	40.492	30.145	11.606	1.00 64.58
ATOM	1972	OW0	WAT	G	190	67.625	60.042	8.441	1.00 33.03
ATOM	1973	OW0	WAT	G	191	50.314	57.576	44.671	1.00 50.98
ATOM	1974	OW0	WAT	G	192	52.073	26.847	-2.175	1.00 30.83
ATOM	1975	OW0	WAT	G	193	46.545	20.307	1.167	1.00 32.08
ATOM	1976	OW0	WAT	G	194	73.086	39.913	40.981	1.00 33.57
ATOM	1977	OW0	WAT	G	195	45.430	39.245	-2.273	1.00 37.02
ATOM	1978	OW0	WAT	G	196	52.037	58.706	12.556	1.00 43.96
ATOM	1979	OW0	WAT	G	197	57.543	61.063	30.828	1.00 37.03
ATOM	1980	OW0	WAT	G	198	61.990	41.753	42.998	1.00 33.81
ATOM	1981	OW0	WAT	G	199	43.339	30.612	18.051	1.00 41.32
ATOM	1982	OW0	WAT	G	200	67.423	56.983	24.190	1.00 29.95
ATOM	1983	OW0	WAT	G	201	63.945	61.652	12.824	1.00 34.11
ATOM	1984	OW0	WAT	G	202	63.921	52.785	39.204	1.00 38.19
ATOM	1985	OW0	WAT	G	203	52.495	20.862	-0.923	1.00 33.05
ATOM	1986	OW0	WAT	G	204	53.126	35.768	-3.356	1.00 51.51
ATOM	1987	OW0	WAT	G	205	42.327	41.556	31.448	1.00 30.36
ATOM	1988	OW0	WAT	G	206	42.439	21.980	7.095	1.00 40.12
ATOM	1989	OW0	WAT	G	207	72.241	46.621	16.496	1.00 54.53
ATOM	1990	OW0	WAT	G	208	74.161	48.453	34.505	1.00 32.75
ATOM	1991	OW0	WAT	G	209	48.098	26.277	-4.627	1.00 41.33
ATOM	1992	OW0	WAT	G	210	70.983	44.677	42.814	1.00 43.40
ATOM	1993	OW0	WAT	G	211	47.557	20.513	-1.605	1.00 40.08
ATOM	1994	OW0	WAT	G	212	61.375	59.056	-0.566	1.00 39.28
ATOM	1995	OW0	WAT	G	213	72.365	48.660	2.612	1.00 35.85
ATOM	1996	OW0	WAT	G	214	42.447	46.142	17.219	1.00 28.95
ATOM	1997	OW0	WAT	G	215	70.417	41.828	12.236	1.00 60.99
ATOM	1998	OW0	WAT	G	216	65.658	40.114	42.603	1.00 38.52
ATOM	1999	OW0	WAT	G	217	61.676	48.645	44.176	1.00 39.02
ATOM	2000	OW0	WAT	G	218	40.044	49.688	1.595	1.00 34.19
ATOM	2001	OW0	WAT	G	219	40.202	42.880	25.589	1.00 32.08
ATOM	2002	OW0	WAT	G	220	70.759	53.406	19.605	1.00 41.25
ATOM	2003	OW0	WAT	G	221	34.228	33.047	11.879	1.00 38.87
ATOM	2004	OW0	WAT	G	222	60.879	55.070	40.559	1.00 33.10
ATOM	2005	OW0	WAT	G	223	58.520	33.967	42.655	1.00 52.56
ATOM	2006	OW0	WAT	G	224	47.130	35.676	-4.383	1.00 40.47
ATOM	2007	OW0	WAT	G	225	42.291	57.764	7.951	1.00 34.20
ATOM	2008	OW0	WAT	G	226	51.783	38.556	-5.023	1.00 54.27
ATOM	2009	OW0	WAT	G	227	63.204	39.780	41.589	1.00 26.92
ATOM	2010	OW0	WAT	G	228	70.115	41.265	21.543	1.00 54.51
ATOM	2011	OW0	WAT	G	229	35.142	41.094	15.033	1.00 26.43
ATOM	2012	OW0	WAT	G	230	49.437	28.507	-7.487	1.00 36.06
ATOM	2013	OW0	WAT	G	231	48.186	58.600	27.989	1.00 47.86
ATOM	2014	OW0	WAT	G	232	43.227	57.642	34.042	1.00 64.53
ATOM	2015	OW0	WAT	G	233	44.435	45.324	40.354	1.00 38.94
ATOM	2016	OW0	WAT	G	234	68.332	40.178	22.530	1.00 41.49
ATOM	2017	OW0	WAT	G	235	41.021	47.384	26.519	1.00 32.18
ATOM	2018	OW0	WAT	G	236	67.943	34.804	44.311	1.00 40.51
ATOM	2019	OW0	WAT	G	237	54.009	33.505	14.576	1.00 38.62
ATOM	2020	OW0	WAT	G	238	69.128	52.076	1.540	1.00 44.17
ATOM	2021	OW0	WAT	G	239	48.173	55.704	43.334	1.00 38.16
ATOM	2022	OW0	WAT	G	240	43.506	19.874	8.570	1.00 34.50
ATOM	2023	OW0	WAT	G	241	46.783	19,606	10.993	1.00 33.70

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ATOM   2024  OW0 WAT G 242      62.052  46.130  46.425  1.00 52.48
ATOM   2025  OW0 WAT G 243      34.174  43.821  10.769  1.00 40.93
ATOM   2026  OW0 WAT G 244      39.585  37.127  26.006  1.00 35.75
ATOM   2027  OW0 WAT G 245      70.915  52.471  29.511  1.00 46.35
ATOM   2028  OW0 WAT G 246      50.280  28.842  -2.906  1.00 34.56
ATOM   2029  OW0 WAT G 247      45.574  23.804  -6.012  1.00 54.66
ATOM   2030  OW0 WAT G 248      50.575  41.649  -5.114  1.00 37.19
ATOM   2031  OW0 WAT G 249      46.284  60.877  -0.658  1.00 48.34
ATOM   2032  OW0 WAT G 250      69.052  41.253  44.563  1.00 41.98
ATOM   2033  OW0 WAT G 251      76.192  44.065  31.740  1.00 39.19
ATOM   2034  OW0 WAT G 252      55.206  59.668   2.632  1.00 44.08
ATOM   2035  OW0 WAT G 253      46.669  36.720  40.608  1.00 50.14
ATOM   2036  OW0 WAT G 254      59.034  52.468  41.277  1.00 35.99
ATOM   2037  OW0 WAT G 255      52.334  63.688  32.421  1.00 64.26
ATOM   2038  OW0 WAT G 256      45.249  20.912  12.682  1.00 45.78
ATOM   2039  OW0 WAT G 257      45.580  47.063  38.611  1.00 32.72
ATOM   2040  OW0 WAT G 258      60.934  36.503  20.702  1.00 58.02
ATOM   2041  OW0 WAT G 259      47.948  47.662  45.709  1.00 33.97
ATOM   2042  OW0 WAT G 260      60.178  62.958   9.683  1.00 36.71
ATOM   2043  OW0 WAT G 261      55.919  30.766  39.029  1.00 61.42
ATOM   2044  OW0 WAT G 262      58.188  56.854  32.396  1.00 36.54
ATOM   2045  OW0 WAT G 263      56.797  37.074  18.930  1.00 61.43
ATOM   2046  OW0 WAT G 264      54.847  38.394  -5.215  1.00 61.42
ATOM   2047  OW0 WAT G 265      74.299  44.365   9.183  1.00 48.11
ATOM   2048  OW0 WAT G 266      68.666  37.135  44.386  1.00 49.26
ATOM   2049  OW0 WAT G 267      48.423  62.166   9.434  1.00 37.66
ATOM   2050  OW0 WAT G 268      42.729  27.614  12.002  1.00 46.39
ATOM   2051  OW0 WAT G 269      53.863  61.181  11.430  1.00 60.41
ATOM   2052  OW0 WAT G 270      65.415  58.143  25.828  1.00 41.48
ATOM   2053  OW0 WAT G 271      51.875  32.393  -8.603  1.00 53.80
ATOM   2054  OW0 WAT G 272      60.962  61.993  12.376  1.00 29.89
ATOM   2055  OW0 WAT G 273      40.308  32.786  11.451  1.00 35.54
ATOM   2056  OW0 WAT G 274      62.383  60.257  17.773  1.00 38.70
ATOM   2057  OW0 WAT G 275      37.093  30.464  14.199  1.00 47.27
ATOM   2058  OW0 WAT G 276      53.952  61.207  -1.317  1.00 46.85
ATOM   2059  OW0 WAT G 277      51.860  29.501   0.746  1.00 37.36
ATOM   2060  OW0 WAT G 278      50.151  63.360   7.446  1.00 45.00
ATOM   2061  OW0 WAT G 279      69.694  43.050  22.397  1.00 68.19
ATOM   2062  OW0 WAT G 280      49.754  37.037  -4.944  1.00 69.60
ATOM   2063  OW0 WAT G 281      50.342  25.060  -3.761  1.00 44.24
ATOM   2064  OW0 WAT G 282      54.321  59.856  16.427  1.00 35.71
ATOM   2065  OW0 WAT G 283      63.746  59.693   0.468  1.00 55.15
ATOM   2066  OW0 WAT G 284      43.389  46.275  36.615  1.00 37.96
ATOM   2067  OW0 WAT G 285      59.808  40.715  43.590  1.00 33.32
ATOM   2068  OW0 WAT G 286      43.995  23.232  16.324  1.00 38.95
ATOM   2069  OW0 WAT G 287      43.552  24.401  13.416  1.00 61.34
ATOM   2070  OW0 WAT G 288      71.661  53.820  27.764  1.00 45.96
ATOM   2071  OW0 WAT G 289      48.871  35.713  37.068  1.00 21.32
ATOM   2072  OW0 WAT G 290      39.975  49.726   8.734  1.00 46.02
ATOM   2074  OW0 WAT G 292      65.526  33.873  35.894  1.00 37.27
ATOM   2075  OW0 WAT G 293      48.218  18.217   9.649  1.00 32.19
ATOM   1783  OW0 WAT H   1      55.626  26.415  10.047  1.00 12.46
ATOM   1784  OW0 WAT H   2      65.016  37.930  11.810  1.00 14.50
ATOM   1785  OW0 WAT H   3      58.211  27.718  10.696  1.00 12.96
ATOM   1786  OW0 WAT H   4      59.947  34.093  10.106  1.00 16.21
ATOM   1787  OW0 WAT H   5      59.936  14.419  20.886  1.00 16.96
ATOM   1788  OW0 WAT H   6      68.238  32.497  17.320  1.00 12.78
ATOM   1789  OW0 WAT H   7      66.240  31.436  15.575  1.00 14.43
ATOM   1790  OW0 WAT H   8      57.265  23.951  22.829  1.00 11.87
ATOM   1791  OW0 WAT H   9      59.422  15.438  31.322  1.00 15.75
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ATOM	1792	OW0	WAT	H	10	64.148	29.630	16.216	1.00	18.14
ATOM	1793	OW0	WAT	H	11	53.858	30.989	20.763	1.00	18.49
ATOM	1794	OW0	WAT	H	12	40.207	30.360	27.502	1.00	20.49
ATOM	1795	OW0	WAT	H	13	52.543	26.702	0.370	1.00	15.58
ATOM	1796	OW0	WAT	H	14	59.344	26.117	22.867	1.00	12.77
ATOM	1797	OW0	WAT	H	15	63.620	27.796	18.221	1.00	17.15
ATOM	1798	OW0	WAT	H	16	70.586	38.510	27.896	1.00	18.45
ATOM	1799	OW0	WAT	H	17	61.696	33.858	24.218	1.00	20.08
ATOM	1800	OW0	WAT	H	18	55.336	28.435	17.716	1.00	19.24
ATOM	1801	OW0	WAT	H	19	62.319	14.684	27.239	1.00	18.83
ATOM	1802	OW0	WAT	H	20	42.537	26.828	34.990	1.00	17.45
ATOM	1803	OW0	WAT	H	21	74.567	31.356	15.807	1.00	18.93
ATOM	1804	OW0	WAT	H	22	77.241	37.609	-1.173	1.00	16.89
ATOM	1805	OW0	WAT	H	23	53.542	26.069	21.187	1.00	20.32
ATOM	1806	OW0	WAT	H	24	78.587	36.637	5.376	1.00	19.88
ATOM	1807	OW0	WAT	H	25	62.185	13.724	24.633	1.00	17.12
ATOM	1808	OW0	WAT	H	26	56.499	11.903	12.602	1.00	21.81
ATOM	1809	OW0	WAT	H	27	49.927	32.676	21.964	1.00	15.81
ATOM	1810	OW0	WAT	H	28	76.722	38.573	6.596	1.00	21.31
ATOM	1811	OW0	WAT	H	29	71.211	17.670	-4.123	1.00	21.20
ATOM	1812	OW0	WAT	H	30	55.890	27.326	15.037	1.00	21.50
ATOM	1813	OW0	WAT	H	31	72.135	13.499	35.278	1.00	26.79
ATOM	1814	OW0	WAT	H	32	76.219	22.099	0.994	1.00	18.33
ATOM	1815	OW0	WAT	H	33	77.438	30.353	-6.384	1.00	21.45
ATOM	1816	OW0	WAT	H	34	75.784	39.054	0.788	1.00	19.77
ATOM	1817	OW0	WAT	H	35	59.941	30.965	22.565	1.00	19.13
ATOM	1818	OW0	WAT	H	36	80.041	33.464	22.515	1.00	25.88
ATOM	1819	OW0	WAT	H	37	53.875	11.516	16.737	1.00	24.35
ATOM	1820	OW0	WAT	H	38	48.562	15.769	23.928	1.00	21.53
ATOM	1821	OW0	WAT	H	39	67.622	19.468	-6.676	1.00	17.05
ATOM	1822	OW0	WAT	H	40	63.265	9.904	29.834	1.00	26.29
ATOM	1823	OW0	WAT	H	41	70.165	13.648	3.894	1.00	26.19
ATOM	1824	OW0	WAT	H	42	81.980	32.799	3.642	1.00	21.59
ATOM	1825	OW0	WAT	H	43	64.411	12.168	24.457	1.00	28.13
ATOM	1826	OW0	WAT	H	44	71.862	38.226	21.699	1.00	27.79
ATOM	1827	OW0	WAT	H	45	50.750	14.483	26.561	1.00	22.42
ATOM	1828	OW0	WAT	H	46	72.225	30.904	-7.142	1.00	24.58
ATOM	1829	OW0	WAT	H	47	48.426	17.990	14.644	1.00	24.59
ATOM	1830	OW0	WAT	H	48	69.915	12.402	20.671	1.00	34.46
ATOM	1831	OW0	WAT	H	49	71.391	27.373	-10.407	1.00	20.52
ATOM	1832	OW0	WAT	H	50	57.327	36.972	-1.991	1.00	29.82
ATOM	1833	OW0	WAT	H	51	68.614	17.512	-4.674	1.00	22.18
ATOM	1834	OW0	WAT	H	52	41.134	22.037	30.497	1.00	17.35
ATOM	1835	OW0	WAT	H	53	78.961	22.828	0.870	1.00	19.50
ATOM	1836	OW0	WAT	H	54	81.114	32.952	25.218	1.00	27.87
ATOM	1837	OW0	WAT	H	55	66.620	38.253	21.637	1.00	30.16
ATOM	1838	OW0	WAT	H	56	82.397	27.950	21.632	1.00	26.01
ATOM	1839	OW0	WAT	H	57	40.601	24.059	32.268	1.00	23.54
ATOM	1840	OW0	WAT	H	58	68.703	17.093	14.330	1.00	30.99
ATOM	1841	OW0	WAT	H	59	60.386	31.945	11.769	1.00	20.83
ATOM	1842	OW0	WAT	H	60	58.159	32.811	23.887	1.00	21.39
ATOM	1843	OW0	WAT	H	61	75.112	33.510	-7.627	1.00	24.77
ATOM	1844	OW0	WAT	H	62	60.861	28.219	17.129	1.00	25.45
ATOM	1845	OW0	WAT	H	63	69.818	18.540	-8.213	1.00	22.75
ATOM	1846	OW0	WAT	H	64	47.698	23.429	29.143	1.00	21.96
ATOM	1847	OW0	WAT	H	65	56.243	17.811	6.113	1.00	26.57
ATOM	1848	OW0	WAT	H	66	56.480	9.527	25.120	1.00	24.57
ATOM	1849	OW0	WAT	H	67	76.416	39.671	4.015	1.00	22.95
ATOM	1850	OW0	WAT	H	68	75.867	11.960	24.892	1.00	26.76
ATOM	1851	OW0	WAT	H	69	65.809	34.125	14.364	1.00	26.61

ATOM	1852	OW0	WAT	H	70	62.222	28.978	20.512	1.00	20.01
ATOM	1853	OW0	WAT	H	71	73.295	41.829	-3.122	1.00	36.97
ATOM	1854	OW0	WAT	H	72	72.362	37.161	14.937	1.00	29.26
ATOM	1855	OW0	WAT	H	73	64.102	12.708	12.209	1.00	29.45
ATOM	1856	OW0	WAT	H	74	59.337	46.991	-4.704	1.00	33.14
ATOM	1857	OW0	WAT	H	75	47.640	15.287	17.293	1.00	25.03
ATOM	1858	OW0	WAT	H	76	65.153	12.787	16.407	1.00	36.34
ATOM	1859	OW0	WAT	H	77	82.754	33.641	27.870	1.00	33.66
ATOM	1860	OW0	WAT	H	78	74.515	43.172	1.368	1.00	46.06
ATOM	1861	OW0	WAT	H	79	65.544	13.826	36.090	1.00	26.95
ATOM	1862	OW0	WAT	H	80	56.176	14.705	7.899	1.00	25.17
ATOM	1863	OW0	WAT	H	81	60.069	12.784	23.279	1.00	25.41
ATOM	1864	OW0	WAT	H	82	64.518	29.497	-9.881	1.00	28.19
ATOM	1865	OW0	WAT	H	83	72.890	17.016	38.513	1.00	32.75
ATOM	1866	OW0	WAT	H	84	64.327	12.726	7.904	1.00	28.33
ATOM	1867	OW0	WAT	H	85	73.702	28.506	40.368	1.00	35.95
ATOM	1868	OW0	WAT	H	86	40.325	34.760	26.876	1.00	30.16
ATOM	1869	OW0	WAT	H	87	46.523	14.958	21.845	1.00	28.34
ATOM	1870	OW0	WAT	H	88	81.785	35.984	25.164	1.00	45.57
ATOM	1871	OW0	WAT	H	89	81.670	23.684	31.981	1.00	30.95
ATOM	1872	OW0	WAT	H	90	73.658	13.615	21.783	1.00	31.75
ATOM	1873	OW0	WAT	H	91	54.962	28.237	22.077	1.00	26.64
ATOM	1874	OW0	WAT	H	92	65.997	21.795	41.162	1.00	34.61
ATOM	1875	OW0	WAT	H	93	67.430	9.979	25.531	1.00	30.41
ATOM	1876	OW0	WAT	H	94	76.456	16.928	20.650	1.00	30.22
ATOM	1877	OW0	WAT	H	95	77.973	22.449	11.319	1.00	26.47
ATOM	1878	OW0	WAT	H	96	54.232	11.639	13.975	1.00	24.52
ATOM	1879	OW0	WAT	H	97	46.826	33.800	36.880	1.00	25.58
ATOM	1880	OW0	WAT	H	98	57.623	16.748	1.335	1.00	35.83
ATOM	1881	OW0	WAT	H	99	60.463	23.883	-10.911	1.00	31.62
ATOM	1882	OW0	WAT	H	100	75.659	24.956	37.083	1.00	35.13
ATOM	1883	OW0	WAT	H	101	59.265	28.532	21.715	1.00	25.37
ATOM	1884	OW0	WAT	H	102	50.039	16.328	12.141	1.00	22.49
ATOM	1885	OW0	WAT	H	103	48.949	27.390	19.574	1.00	22.74
ATOM	1886	OW0	WAT	H	104	52.769	29.349	16.776	1.00	23.17
ATOM	1887	OW0	WAT	H	105	57.967	25.041	-7.141	1.00	29.64
ATOM	1888	OW0	WAT	H	106	75.831	28.016	37.410	1.00	34.04
ATOM	1889	OW0	WAT	H	107	77.822	15.717	-6.480	1.00	35.09
ATOM	1890	OW0	WAT	H	108	65.905	16.140	14.395	1.00	25.94
ATOM	1891	OW0	WAT	H	109	52.151	13.189	12.986	1.00	26.50
ATOM	1892	OW0	WAT	H	110	80.013	37.977	7.957	1.00	30.56
ATOM	1893	OW0	WAT	H	111	83.151	30.502	29.885	1.00	29.70
ATOM	1894	OW0	WAT	H	112	70.714	15.340	37.184	1.00	35.84
ATOM	1895	OW0	WAT	H	113	62.628	31.924	-7.181	1.00	30.25
ATOM	1896	OW0	WAT	H	114	50.066	27.262	16.994	1.00	30.45
ATOM	1897	OW0	WAT	H	115	45.810	22.478	26.282	1.00	30.65
ATOM	1898	OW0	WAT	H	116	39.755	32.861	30.859	1.00	26.85
ATOM	1899	OW0	WAT	H	117	71.066	9.044	35.678	1.00	36.26
ATOM	1900	OW0	WAT	H	118	58.464	30.897	-6.302	1.00	33.36
ATOM	1901	OW0	WAT	H	119	43.885	38.361	32.035	1.00	39.06
ATOM	1902	OW0	WAT	H	120	48.283	14.313	19.784	1.00	23.39
ATOM	1903	OW0	WAT	H	121	58.695	11.110	24.826	1.00	32.00
ATOM	1904	OW0	WAT	H	122	57.082	19.459	-4.887	1.00	28.95
ATOM	1905	OW0	WAT	H	123	81.562	27.571	7.690	1.00	31.43
ATOM	1906	OW0	WAT	H	124	50.133	7.422	22.846	1.00	30.11
ATOM	1907	OW0	WAT	H	125	69.527	37.104	15.998	1.00	37.52
ATOM	1908	OW0	WAT	H	126	83.637	20.159	29.764	1.00	30.85
ATOM	1909	OW0	WAT	H	127	57.160	30.346	18.132	1.00	28.43
ATOM	1910	OW0	WAT	H	128	55.407	22.216	37.933	1.00	28.17
ATOM	1911	OW0	WAT	H	129	39.281	32.022	33.251	1.00	36.60

ATOM	1912	OW0	WAT	H	130	66.017	13.623	13.755	1.00 29.95
ATOM	1913	OW0	WAT	H	131	78.517	19.411	5.018	1.00 29.87
ATOM	1914	OW0	WAT	H	132	48.811	17.945	26.897	1.00 43.00
ATOM	1917	OW0	WAT	H	135	64.367	34.584	23.669	1.00 15.27
ATOM	1918	OW0	WAT	H	136	81.580	19.230	1.174	1.00 23.04
ATOM	1919	OW0	WAT	H	137	60.573	29.499	14.716	1.00 20.63
ATOM	1920	OW0	WAT	H	138	65.862	34.058	21.256	1.00 34.20
ATOM	1921	OW0	WAT	H	139	83.247	24.263	5.613	1.00 31.10
ATOM	1922	OW0	WAT	H	140	59.546	29.382	19.222	1.00 26.78
ATOM	1923	OW0	WAT	H	141	57.588	28.862	13.258	1.00 28.89
ATOM	1924	OW0	WAT	H	142	67.042	36.289	15.327	1.00 30.25
ATOM	1925	OW0	WAT	H	143	79.364	24.456	-3.023	1.00 27.10
ATOM	1926	OW0	WAT	H	144	56.647	25.991	39.022	1.00 24.20
ATOM	1927	OW0	WAT	H	145	56.593	34.283	22.128	1.00 27.16
ATOM	1928	OW0	WAT	H	146	73.331	26.272	-7.226	1.00 27.11
ATOM	1929	OW0	WAT	H	147	47.705	20.384	15.670	1.00 27.47
ATOM	1930	OW0	WAT	H	148	75.910	26.130	-7.246	1.00 29.71
ATOM	1931	OW0	WAT	H	149	46.323	26.826	19.400	1.00 36.67
ATOM	1932	OW0	WAT	H	150	61.609	39.798	2.091	1.00 30.16
ATOM	1933	OW0	WAT	H	151	68.189	35.212	17.395	1.00 28.63
ATOM	1934	OW0	WAT	H	152	49.690	27.733	40.873	1.00 26.64
ATOM	1935	OW0	WAT	H	153	81.739	25.115	8.578	1.00 34.13
ATOM	1936	OW0	WAT	H	154	64.261	33.918	17.410	1.00 48.10
ATOM	1937	OW0	WAT	H	155	55.864	32.706	19.968	1.00 40.67
ATOM	1938	OW0	WAT	H	156	62.576	31.794	17.551	1.00 34.94
ATOM	1939	OW0	WAT	H	157	52.628	31.942	-3.590	1.00 38.68
ATOM	1940	OW0	WAT	H	158	75.447	17.848	6.325	1.00 25.79
ATOM	1941	OW0	WAT	H	159	59.047	22.586	38.987	1.00 29.14
ATOM	1942	OW0	WAT	H	160	59.817	35.142	14.016	1.00 38.25
ATOM	1943	OW0	WAT	H	161	78.322	14.589	40.993	1.00 32.32
ATOM	1944	OW0	WAT	H	162	57.184	22.624	-0.720	1.00 28.29
ATOM	1945	OW0	WAT	H	163	61.680	31.893	20.126	1.00 45.25
ATOM	1946	OW0	WAT	H	164	48.637	24.862	17.484	1.00 28.59
ATOM	1947	OW0	WAT	H	165	67.349	36.023	19.750	1.00 36.40
ATOM	1948	OW0	WAT	H	166	80.275	22.814	34.316	1.00 36.57
ATOM	1949	OW0	WAT	H	167	80.632	18.004	27.037	1.00 35.99
ATOM	1950	OW0	WAT	H	168	61.282	32.543	14.506	1.00 46.77
ATOM	1951	OW0	WAT	H	169	74.823	41.370	-0.405	1.00 28.55
ATOM	1952	OW0	WAT	H	170	77.282	27.797	-5.491	1.00 28.32
ATOM	1953	OW0	WAT	H	171	65.084	44.653	-1.597	1.00 27.69
ATOM	1954	OW0	WAT	H	172	63.688	35.041	21.190	1.00 50.53
ATOM	1955	OW0	WAT	H	173	82.147	28.336	34.535	1.00 31.26
ATOM	1956	OW0	WAT	H	174	68.214	48.464	-1.584	1.00 35.85
ATOM	1957	OW0	WAT	H	175	74.240	41.773	10.211	1.00 36.58
ATOM	1958	OW0	WAT	H	176	70.408	35.424	18.373	1.00 40.37
ATOM	1959	OW0	WAT	H	177	68.932	38.086	20.571	1.00 42.76
ATOM	1960	OW0	WAT	H	178	81.267	16.180	3.373	1.00 53.70
ATOM	1961	OW0	WAT	H	179	68.820	19.728	-13.191	1.00 29.11
ATOM	1962	OW0	WAT	H	180	54.827	19.858	30.125	1.00 33.03
ATOM	1963	OW0	WAT	H	181	77.490	36.105	18.544	1.00 35.32
ATOM	1964	OW0	WAT	H	182	81.400	31.344	21.170	1.00 27.00
ATOM	1965	OW0	WAT	H	183	78.807	41.819	9.585	1.00 39.70
ATOM	1966	OW0	WAT	H	184	55.707	34.988	-1.978	1.00 43.06
ATOM	1967	OW0	WAT	H	185	69.768	32.598	-7.874	1.00 32.67
ATOM	1968	OW0	WAT	H	186	75.082	37.972	15.406	1.00 37.29
ATOM	1969	OW0	WAT	H	187	84.025	26.790	23.695	1.00 28.47
ATOM	1970	OW0	WAT	H	188	72.505	36.365	17.754	1.00 53.73
ATOM	1971	OW0	WAT	H	189	46.352	19.994	24.180	1.00 64.58
ATOM	1972	OW0	WAT	H	190	85.809	28.542	27.345	1.00 33.03
ATOM	1973	OW0	WAT	H	191	75.018	14.784	-8.885	1.00 50.98

ATOM	1974	OW0	WAT	H	192	49.286	31.672	37.961	1.00	30.83
ATOM	1975	OW0	WAT	H	193	40.858	30.154	34.619	1.00	32.08
ATOM	1976	OW0	WAT	H	194	71.108	43.336	-5.195	1.00	33.57
ATOM	1977	OW0	WAT	H	195	56.701	19.720	38.059	1.00	37.02
ATOM	1978	OW0	WAT	H	196	76.858	15.711	23.230	1.00	43.96
ATOM	1979	OW0	WAT	H	197	81.652	19.301	4.958	1.00	37.03
ATOM	1980	OW0	WAT	H	198	67.153	32.807	-7.212	1.00	33.81
ATOM	1981	OW0	WAT	H	199	48.179	22.226	17.735	1.00	41.32
ATOM	1982	OW0	WAT	H	200	83.059	29.897	11.596	1.00	29.95
ATOM	1983	OW0	WAT	H	201	85.363	24.550	22.962	1.00	34.11
ATOM	1984	OW0	WAT	H	202	77.672	28.963	-3.418	1.00	38.19
ATOM	1985	OW0	WAT	H	203	44.314	35.030	36.709	1.00	33.05
ATOM	1986	OW0	WAT	H	204	57.538	28.123	39.142	1.00	51.51
ATOM	1987	OW0	WAT	H	205	57.151	15.877	4.338	1.00	30.36
ATOM	1988	OW0	WAT	H	206	40.254	25.762	28.691	1.00	40.12
ATOM	1989	OW0	WAT	H	207	76.494	39.250	19.290	1.00	54.53
ATOM	1990	OW0	WAT	H	208	79.041	39.997	1.281	1.00	32.75
ATOM	1991	OW0	WAT	H	209	46.805	28.514	40.413	1.00	41.33
ATOM	1992	OW0	WAT	H	210	74.182	39.133	-7.028	1.00	43.40
ATOM	1993	OW0	WAT	H	211	41.543	30.928	37.391	1.00	40.08
ATOM	1994	OW0	WAT	H	212	81.830	23.623	36.352	1.00	39.28
ATOM	1995	OW0	WAT	H	213	78.322	38.338	33.174	1.00	35.85
ATOM	1996	OW0	WAT	H	214	61.182	13.688	18.567	1.00	28.95
ATOM	1997	OW0	WAT	H	215	71.432	40.067	23.550	1.00	60.99
ATOM	1998	OW0	WAT	H	216	67.568	36.803	-6.817	1.00	38.52
ATOM	1999	OW0	WAT	H	217	72.965	29.089	-8.390	1.00	39.02
ATOM	2000	OW0	WAT	H	218	63.052	9.834	34.191	1.00	34.19
ATOM	2001	OW0	WAT	H	219	57.235	13.375	10.197	1.00	32.08
ATOM	2002	OW0	WAT	H	220	81.629	34.574	16.181	1.00	41.25
ATOM	2003	OW0	WAT	H	221	45.733	13.118	23.907	1.00	38.87
ATOM	2004	OW0	WAT	H	222	78.130	25.186	-4.773	1.00	33.10
ATOM	2005	OW0	WAT	H	223	58.675	33.695	-6.869	1.00	52.56
ATOM	2006	OW0	WAT	H	224	54.460	22.977	40.169	1.00	40.47
ATOM	2007	OW0	WAT	H	225	71.169	7.742	27.835	1.00	34.20
ATOM	2008	OW0	WAT	H	226	59.281	25.566	40.809	1.00	54.27
ATOM	2009	OW0	WAT	H	227	66.051	34.845	-5.803	1.00	26.92
ATOM	2010	OW0	WAT	H	228	70.793	40.087	14.243	1.00	54.51
ATOM	2011	OW0	WAT	H	229	53.158	9.886	20.753	1.00	26.43
ATOM	2012	OW0	WAT	H	230	49.406	28.559	43.273	1.00	36.06
ATOM	2013	OW0	WAT	H	231	74.841	12.429	7.797	1.00	47.86
ATOM	2014	OW0	WAT	H	232	71.531	8.614	1.744	1.00	64.53
ATOM	2015	OW0	WAT	H	233	61.468	15.819	-4.568	1.00	38.94
ATOM	2016	OW0	WAT	H	234	68.960	39.087	13.256	1.00	41.49
ATOM	2017	OW0	WAT	H	235	61.545	11.832	9.267	1.00	32.18
ATOM	2018	OW0	WAT	H	236	64.112	41.437	-8.525	1.00	40.51
ATOM	2019	OW0	WAT	H	237	56.020	30.019	21.210	1.00	38.62
ATOM	2020	OW0	WAT	H	238	79.662	33.827	34.246	1.00	44.17
ATOM	2021	OW0	WAT	H	239	72.326	13.866	-7.548	1.00	38.16
ATOM	2022	OW0	WAT	H	240	38.964	27.739	27.216	1.00	34.50
ATOM	2023	OW0	WAT	H	241	40.370	30.711	24.793	1.00	33.70
ATOM	2024	OW0	WAT	H	242	70.975	30.672	-10.639	1.00	52.48
ATOM	2025	OW0	WAT	H	243	55.036	7.684	25.017	1.00	40.93
ATOM	2026	OW0	WAT	H	244	51.944	15.717	9.780	1.00	35.75
ATOM	2027	OW0	WAT	H	245	80.897	35.177	6.275	1.00	46.35
ATOM	2028	OW0	WAT	H	246	50.117	29.121	38.692	1.00	34.56
ATOM	2029	OW0	WAT	H	247	43.401	27.565	41.798	1.00	54.66
ATOM	2030	OW0	WAT	H	248	61.356	22.973	40.900	1.00	37.19
ATOM	2031	OW0	WAT	H	249	75.861	9.643	36.444	1.00	48.34
ATOM	2032	OW0	WAT	H	250	70.251	39.173	-8.777	1.00	41.98
ATOM	2033	OW0	WAT	H	251	76.256	43.950	4.046	1.00	39.19

ATOM	2034	OW0	WAT	H	252	79.275	17.974	33.154	1.00	44.08
ATOM	2035	OW0	WAT	H	253	55.134	22.055	-4.822	1.00	50.14
ATOM	2036	OW0	WAT	H	254	74.954	24.889	-5.491	1.00	35.99
ATOM	2037	OW0	WAT	H	255	81.321	13.477	3.365	1.00	64.26
ATOM	2038	OW0	WAT	H	256	40.734	28.730	23.104	1.00	45.78
ATOM	2039	OW0	WAT	H	257	63.547	15.941	-2.825	1.00	32.72
ATOM	2040	OW0	WAT	H	258	62.079	34.517	15.084	1.00	58.02
ATOM	2041	OW0	WAT	H	259	65.249	17.692	-9.923	1.00	33.97
ATOM	2042	OW0	WAT	H	260	84.611	20.635	26.103	1.00	36.71
ATOM	2043	OW0	WAT	H	261	54.603	33.043	-3.243	1.00	61.42
ATOM	2044	OW0	WAT	H	262	78.330	21.964	3.390	1.00	36.54
ATOM	2045	OW0	WAT	H	263	60.505	30.649	16.856	1.00	61.43
ATOM	2046	OW0	WAT	H	264	60.673	28.301	41.001	1.00	61.42
ATOM	2047	OW0	WAT	H	265	75.570	42.160	26.603	1.00	48.11
ATOM	2048	OW0	WAT	H	266	66.492	40.897	-8.600	1.00	49.26
ATOM	2049	OW0	WAT	H	267	78.047	10.851	26.352	1.00	37.66
ATOM	2050	OW0	WAT	H	268	45.278	23.196	23.784	1.00	46.39
ATOM	2051	OW0	WAT	H	269	79.914	16.055	24.356	1.00	60.41
ATOM	2052	OW0	WAT	H	270	83.059	27.578	9.958	1.00	41.48
ATOM	2053	OW0	WAT	H	271	53.990	28.727	44.389	1.00	53.80
ATOM	2054	OW0	WAT	H	272	84.167	21.797	23.410	1.00	29.89
ATOM	2055	OW0	WAT	H	273	48.547	18.514	24.335	1.00	35.54
ATOM	2056	OW0	WAT	H	274	83.374	23.895	18.013	1.00	38.70
ATOM	2057	OW0	WAT	H	275	44.928	16.891	21.587	1.00	47.27
ATOM	2058	OW0	WAT	H	276	79.981	16.119	37.103	1.00	46.85
ATOM	2059	OW0	WAT	H	277	51.478	30.160	35.040	1.00	37.36
ATOM	2060	OW0	WAT	H	278	79.945	11.751	28.340	1.00	45.00
ATOM	2061	OW0	WAT	H	279	72.128	38.830	13.389	1.00	68.19
ATOM	2062	OW0	WAT	H	280	56.951	24.568	40.730	1.00	69.60
ATOM	2063	OW0	WAT	H	281	46.873	31.066	39.547	1.00	44.24
ATOM	2064	OW0	WAT	H	282	78.996	17.114	19.359	1.00	35.71
ATOM	2065	OW0	WAT	H	283	83.567	25.358	35.318	1.00	55.15
ATOM	2066	OW0	WAT	H	284	61.769	14.437	-0.829	1.00	37.96
ATOM	2067	OW0	WAT	H	285	65.163	31.436	-7.804	1.00	33.32
ATOM	2068	OW0	WAT	H	286	42.116	26.484	19.462	1.00	38.95
ATOM	2069	OW0	WAT	H	287	42.907	25.516	22.370	1.00	61.34
ATOM	2070	OW0	WAT	H	288	82.439	35.148	8.022	1.00	45.96
ATOM	2071	OW0	WAT	H	289	55.363	24.466	-1.282	1.00	21.32
ATOM	2072	OW0	WAT	H	290	63.050	9.755	27.052	1.00	46.02
ATOM	2074	OW0	WAT	H	292	62.097	39.809	-0.108	1.00	37.27
ATOM	2075	OW0	WAT	H	293	39.885	32.648	26.137	1.00	32.19

Table 2: Binding sites of the ADC binding cavity (the atomic coordinates of the binding sites are provided in Table 1)

Binding site no.	Amino acid residue	Atom(s) involved	Atom no. in Table 1	Binding interaction
1	Tyr22A	C_{D2}	180	HI
		C_{E2}	182	
2	Pvl25A	C_A	201	CB
3	Pvl25A	C_B	202	HI
4	Thr57A	O_{G1}	450	HB
5	Tyr58A	C_G	457	HI
		C_{E1}	460	
		C_{E2}	461	
		C_{D1}	458	
		C_{D2}	459	
		C_Z	462	
6	Ile60A	C_{G1}	474	HI
		C_{G2}	475	
		C_{D1}	476	
7	Asn72A	O	560	HB
8	Ala75A	N	574	HB
9	Lys9D	N_Z	963	HB, II or SMI
10	Trp47D	C_G	1256	π
		C_{D1}	1257	
		C_{D2}	1258	
		C_{E2}	1260	
		C_{E3}	1261	
		C_{Z2}	1262	
		C_{Z3}	1263	
		C_{H2}	1264	
		N_{E1}	1259	
11	Arg54D	N_{H1}	1317	II
		N_{H2}	1318	

CB = Covalent Bond
HB = Hydrogen Bond
II = Ionic Interaction
HI = Hydrophobic Interaction
π = π Interaction
SMI = Sulphate-Mediated Interaction

Table 3: X-ray crystallographic data quality statistics

	Native	*MeAsp*	*rβAla*	*isoA*	*Sbst*	*Prod*
Space group:			**$P6_122$**			
Wavelength (Å)	0.87	1.54	1.54	1.54	1.54	1.54
Number of frames	360	200	90	90	155	138
2θ angle setting (°)	0	24.3	17.8	0	27.2	19
Resolution (Å)[a]	1.55	1.7	1.9	1.7	1.5	1.7
Estimated mosaicity (°)	0.24	0.36	0.35	0.24	0.31	0.42
No. observed reflexions	1025720	298195	107245	158424	103704	143040
No. unique reflexions	47 479	33 689	24 116	33 723	39 320	32 160
Multiplicity	**8.9**	**8.9**	**4.4**	**4.7**	**2.6**	**4.1**
Completeness (All data) (%)	98.9	93.6	91.9	93.7	76.9	89.2
Completeness (highest resol.) (%)	91.0	88.1	81.1	69.2	63.9	57.2
Low resolution limit (Å)[b]	60	22	11.5	25	10.3	14.8
No. reflexions missing < 10 Å	**16** /247	**48** /244	**99** /246	**21** /245	**219**/246	**17** /246
Average I/σ(I)	24.9	20.5	13.1	23.0	18.7	15.3
I/σ(I) (highest resolution shell)	6.8	2.4	1.7	3.5	2.3	1.8
R_{meas}[c]	0.071	0.064	0.070	0. 048	0.059	0.090
R_{meas} (highest resolution shell)	0.166	0.499	0.590	0.330	0.399	0.382

[a] Judged where I/σ(I) > 2.

[b] Judged where I/σ(I) is largest and R_{meas} lowest.

[c] Multiplicity weighted R_{sym}:

$$R_{meas} = \frac{\sum_{\mathbf{h}} \sqrt{\frac{n_{\mathbf{h}}}{n_{\mathbf{h}}-1}} \sum_{i} \left| \hat{I}_{\mathbf{h}} - I_{\mathbf{h},i} \right|}{\sum_{\mathbf{h}} \sum_{i} I_{\mathbf{h},i}}, \hat{I}_{\mathbf{h}} = \frac{1}{n_{\mathbf{h}}} \sum_{i}^{n_{\mathbf{h}}} I_{\mathbf{h}}$$

Table 4: Model refinement convergence criteria and parameters, and quality indicators.

	Nat	*MeAsp*	*IsoA*	*Prod*	*Subst*	*rβAla*
Crystallographic refinement						
No. reflexions for refinement	44 963	32 355	32 349	30 807	37 582	21 420
No. test reflexions[a]	2 395	1 360	1 348	1 266	1 620	1 657
No. restraints[b]	6 430	6 500	6 491	6 482	6 497	6 473
No. parameters	8 300	8 888	8 832	8 744	8 536	8 220
Weight for geom. restraints (*TNT*)	4	3	4	4	4	3
Final model parameters						
Residues	228	228	228	228	228	228
Hetero groups	2	4	4	4	4	6
No. water molecules	290	422	410	393	336	261
No. non-hydrogen atoms	2 072	2 222	2 208	2 185	2 134	2 063
Resolution range (Å)	60 –1.55	22 – 1.7	11.5–1.7	25 – 1.7	10.3-1.5	14 – 1.9
Refinement convergence						
R_{free}[c]	0.217	0.205	0.196	0.206	0.194	0.229
R_{factor}[d]	0.198	0.176	0.167	0.172	0.177	0.182
Average *B*-factor, subunit A (Å^2)	18.1	23.3	21.1	18.4	20.9	25.8
subunit B(Å^2)	20.7	25.4	23.3	20.1	21.9	29.4
waters (Å)	33.2	46.0	42.9	37.4	36.9	41.0
Wilson distribution B_{factor} (Å^2)	17.8	22.6	21.4	19.7	18.8	23.1
Model quality						
Ramachandran plot:						
% residues						
In most favoured region	91.2	90.7	90.6	91.2	90.6	90.1
In generously allowed region	8.8	9.3	9.4	8.8	9.4	9.9
In disallowed region	0	0	0	0	0	0

RMS[e] deviation from ideal						
Covalent bond lengths (Å)	0.022	0.018	0.021	0.023	0.019	0.018
Bond angles (°)	1.8	1.6	1.9	1.6	1.7	1.5
Planar groups (Å)	0.013	0.015	0.016	0.011	0.012	0.012
Procheck[f] criteria						
Bond length outliers (%)	5.9	2.4	5.2	6.5	3.9	2.2
Bond angle outliers (%)	6.1	4.0	4.8	4.4	5.2	3.8
Planarity outliers (%)	2.3	0	0	2.9	0	0

[a] Test set is excluded from refinement for cross-validation (Brunger, 1992).

[b] Restraints in TNT with non-zero weight.

[c] R_{factor} calculated using test reflexions.

[d] $R_{factor} = \Sigma_h||F_{obs}| - |F_{calc}|| / \Sigma_h|F_{obs}|$, with test reflexions excluded.

[e] RMS – Root mean square

[f] Laskowski *et al.*, 1993

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The references mentioned in the above text and listed below are incorporated by reference.

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Claims

1. A method of identifying an agent compound which modulates asparate decarboxylase (ADC) activity comprising the steps of:

a) providing a model of a binding cavity of ADC, said model including at least one of binding site nos. 1 and 9 defined by Table 2;

b) providing the structure of a candidate agent compound;

c) fitting the candidate agent compound to said binding cavity, including determining the interactions between the candidate agent compound and at least one of binding site nos. 1 and 9; and

d) selecting the fitted candidate agent compound.

2. The method according to claim 1, comprising the further step of:

e) contacting the candidate agent compound with ADC to determine the ability of the candidate agent compound to interact with ADC.

3. The method according to claim 1, comprising the further steps of:

e) forming a complex of ADC and said candidate agent compound; and

f) analysing said complex by X-ray crystallography or NMR spectroscopy to determine the ability of said candidate agent compound to interact with ADC.

4. A crystal of fully processed ADC.

5. A crystal of fully processed ADC having a hexagonal point group 622.

6. A crystal of fully processed ADC having a hexagonal space group $P6_122$.

7. A crystal of ADC which diffracts X-rays for the determination of atomic coordinates of ADC to a resolution of better than 2Å.

8. A crystal of ADC according to claim 7, wherein the ADC is fully processed.

9. A crystal of fully processed ADC having unit cell dimensions of a = 71.1 Å ± 5%, and c = 215.8 Å ± 5%.

10. A crystal of fully processed ADC having the three dimensional atomic coordinates of Table 1.

11. A method of fully processing ADC, comprising the step of forming a solution of ADC, the solution having a pH in the range 6.5-8.5 and an ADC concentration in the range 1-50 mg/ml.

12. A method for growing a crystal of ADC, which method comprises:

forming a 1:1 mixture of a crystallising solution containing 1.6 to 2.4 M $Na_2(SO_4)$ and a protein solution containing ADC at a concentration of 6 to 10 mg/ml in 25 mM HEPES buffer at pH 7.5, and

growing the crystal by vapour diffusion from the mixture.

13. A method of testing a candidate agent compound for ability to modulate ADC activity, comprising the step of contacting the candidate agent compound with fully processed ADC to determine the ability of the candidate agent compound to interact with ADC.

14. A method of identifying an agent compound which modulates ADC activity, comprising the steps of:

a) providing a candidate agent compound;

b) forming a complex of fully processed ADC and the candidate agent compound; and

c) analysing said complex by X-ray crystallography or NMR spectroscopy to determine the ability of the candidate agent compound to interact with ADC.

15. A method of analysing an ADC-ligand complex comprising the step of employing (i) X-ray crystallographic diffraction data from the fully processed ADC-ligand complex and (ii) a three-dimensional structure of fully processed ADC, to generate a difference Fourier electron density map of the complex, the three-dimensional structure being defined by atomic coordinate data according to Table 1.

16. A chimaeric protein having a binding cavities for L-aspartate, the binding cavity providing a plurality of atoms which interact with L-aspartate and which correspond to selected ADC atoms in the ADC binding cavity for L-aspartate, the relative positions of the plurality of atoms corresponding to the relative positions, as defined by Table 1, of the selected ADC atoms,

wherein either or both of binding site nos. 1 and 9 defined by Table 2 provide one or more of the selected ADC atoms

17. A computer system, intended to generate structures and/or perform rational drug design for ADC, or complexes of ADC with a potential modulator; the systems containing computer-readable data comprising at least one of: (a) atomic coordinate data according to Table 1, said data defining the three-dimensional structure of fully processed ADC; and (b) structure factor data for ADC, said structure factor data being derivable from the atomic coordinate data of Table 1.

18. A computer system according to claim 17 comprising:

(i) a computer-readable data storage medium comprising data storage material encoded with the computer-readable data;

(ii) a working memory for storing instructions for processing said computer-readable data; and

(iii) a central-processing unit coupled to said working memory and to said computer-readable data storage medium for processing said computer-readable data and thereby generating structures and/or performing rational drug design

19. Computer readable media with at least one of: (a) atomic coordinate data according to Table 1 recorded thereon, said data defining the three-dimensional structure of fully processed ADC; and (b) structure factor data for ADC recorded thereon, the structure factor data being derivable from the atomic coordinate data of Table 1.

20. A method of providing data for generating structures and/or performing rational drug design for ADC, or complexes of ADC with a potential modulator, the method comprising:

(i) establishing communication with a remote device containing computer-readable data comprising at least one of: (a) atomic coordinate data according to Table 1, said data defining the three-dimensional structure of fully processed ADC; and (b) structure factor data for ADC, said structure factor data being derivable from the atomic coordinate data of Table 1; and

(ii) receiving said computer-readable data from said remote device.

Figure 1

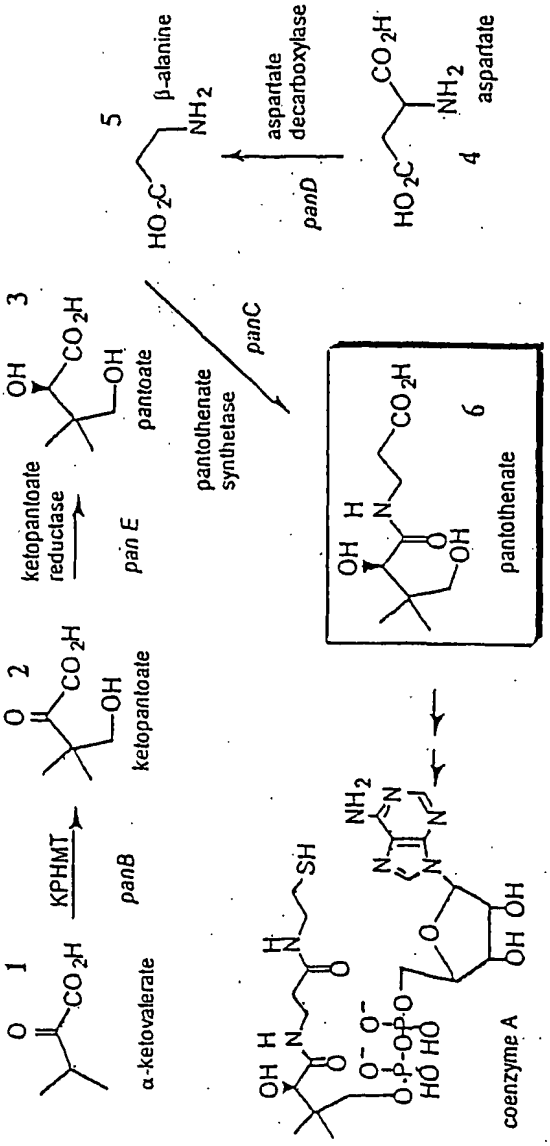

α-ketovalerate
KPHMT
panB
ketopantoate
ketopantoate reductase
pan E
pantoate
pantothenate synthetase
panC
β-alanine
aspartate decarboxylase
panD
aspartate
pantothenate
coenzyme A

Figure 2

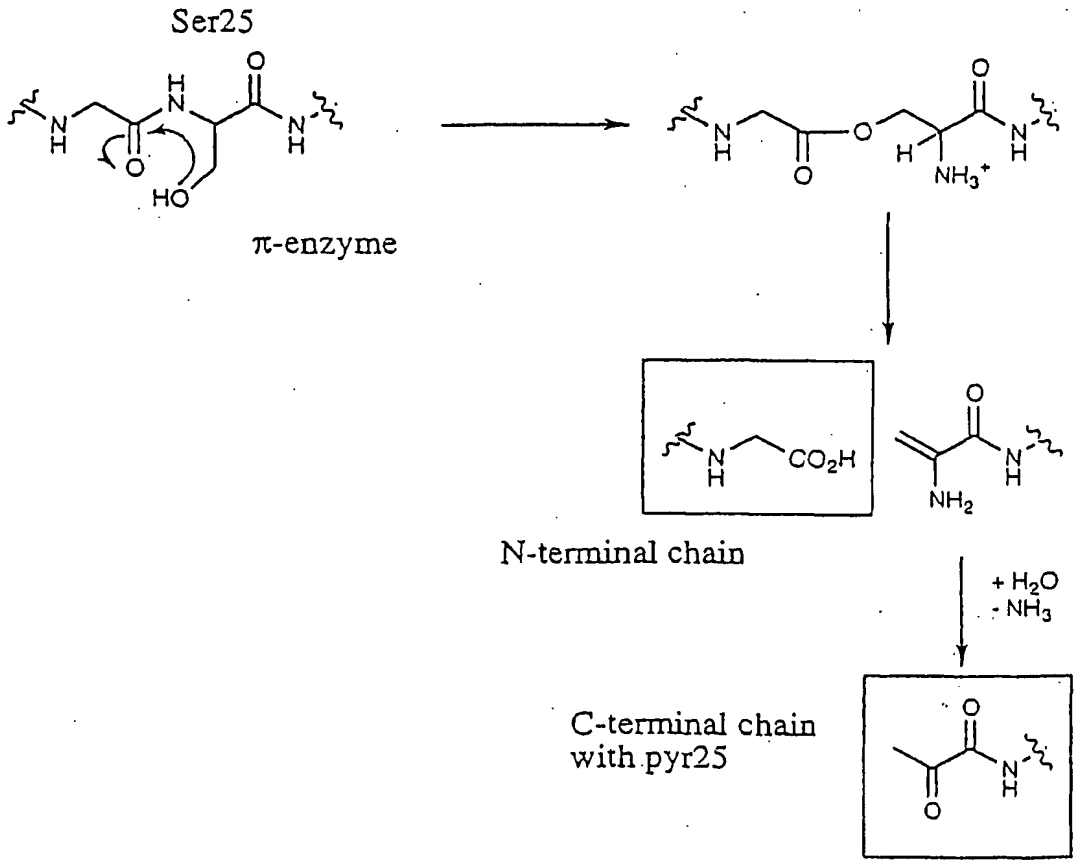
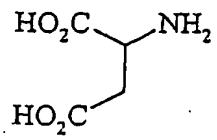

Ser25
π-enzyme
N-terminal chain
C-terminal chain
with pyr25
+ H2O
- NH3

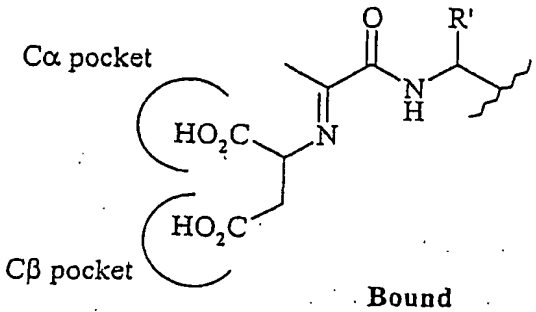
Figure 3a

L-Aspartate (Sbst)



Unbound

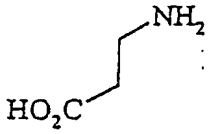
Imine Species



Bound

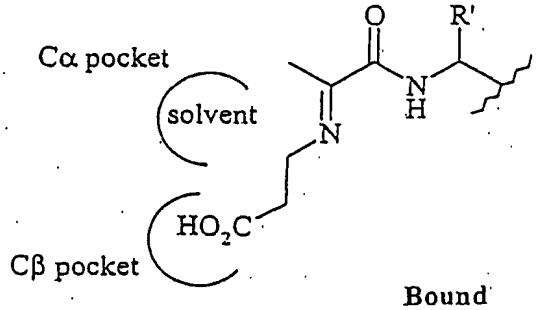
Figure 3b

β-Alanine (Prod)



Unbound

Imine Species

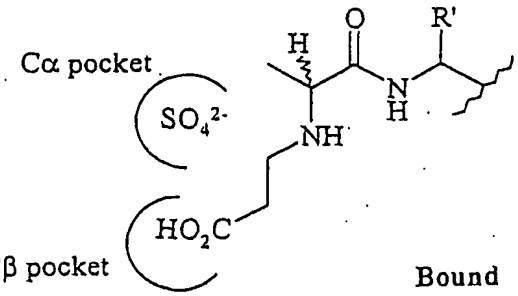


Bound

Figure 3c

Reductively Bound
β-Alanine (rβAla)

Imine Species



Bound

Figure 3d

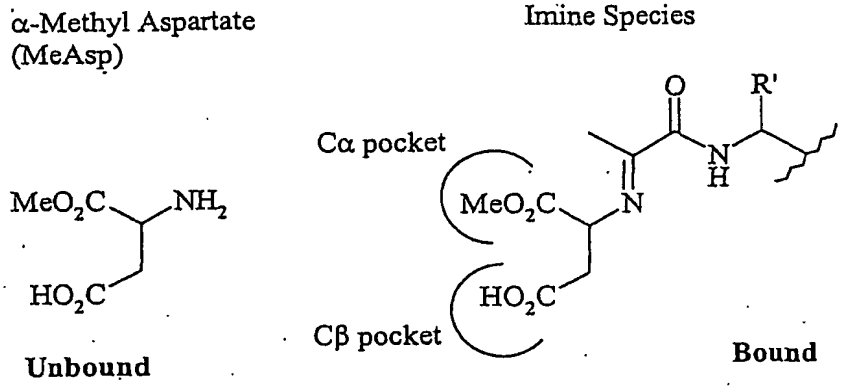


Figure 3e

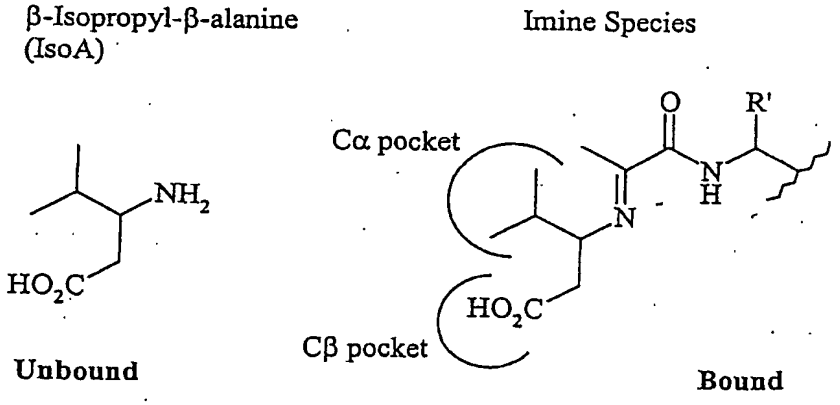


Figure 4

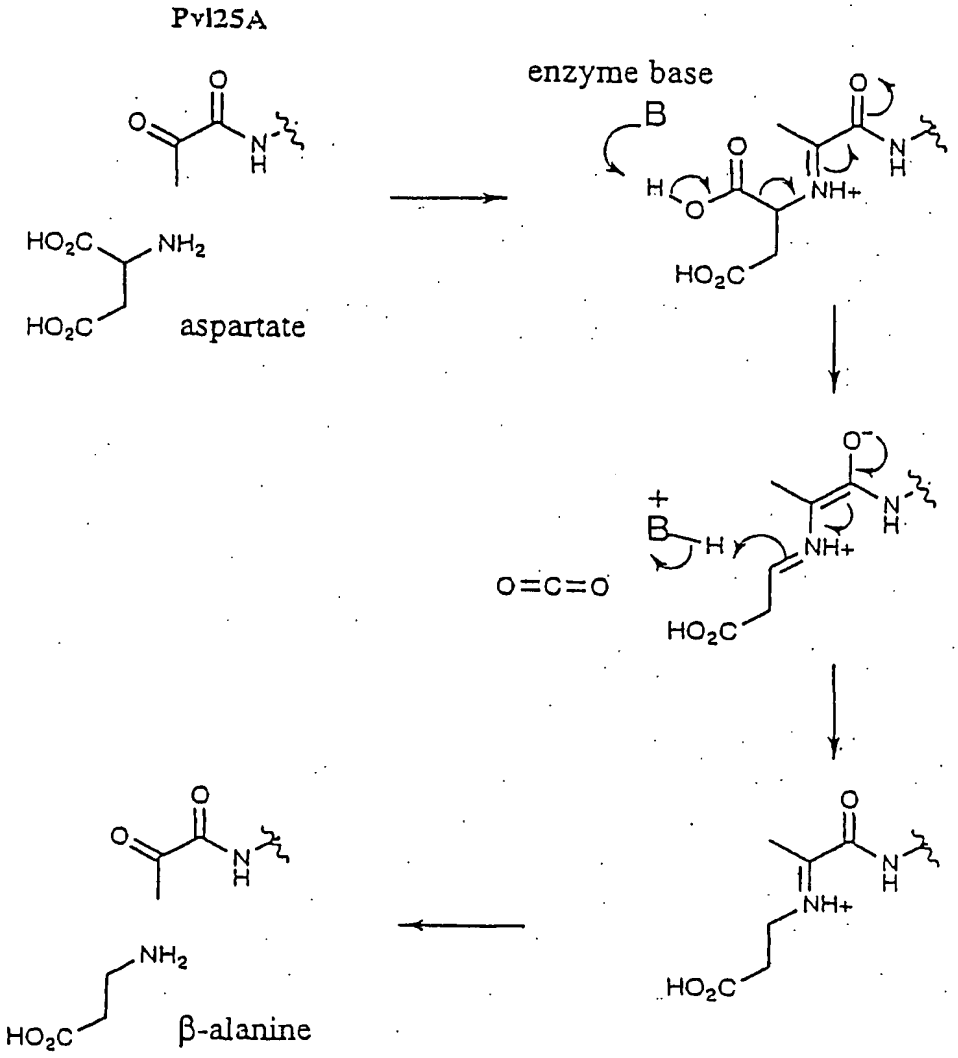

PvI25A
enzyme base
B
H
O
NH+
HO2C
HO2C
NH2
aspartate
O=C=O
β-alanine

Figure 5a

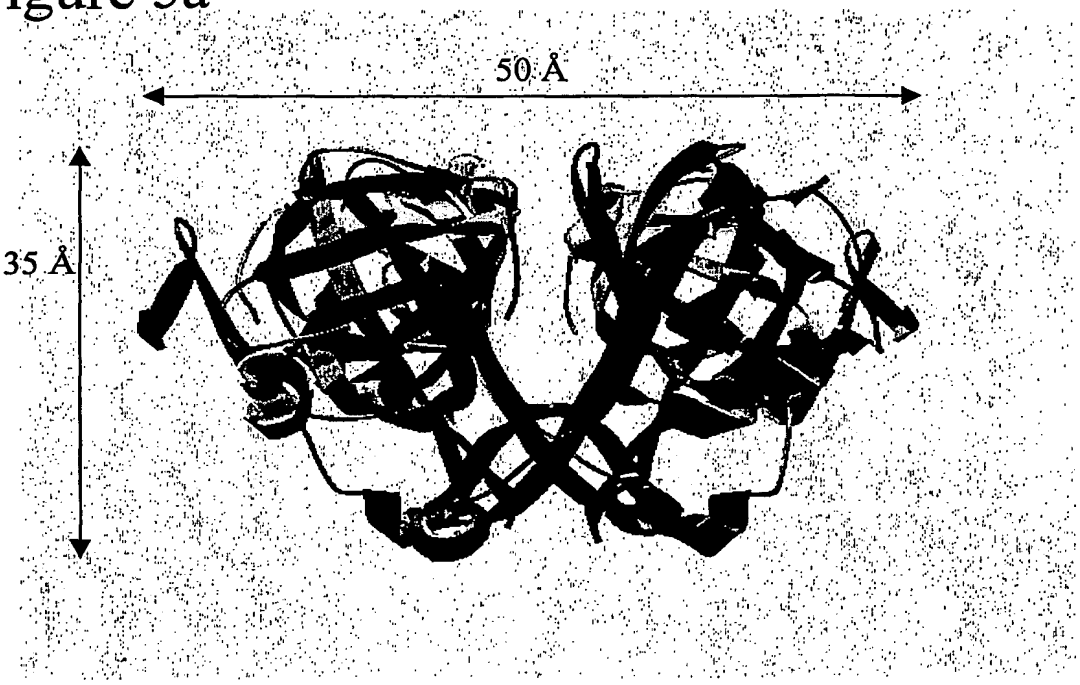


Figure 5b

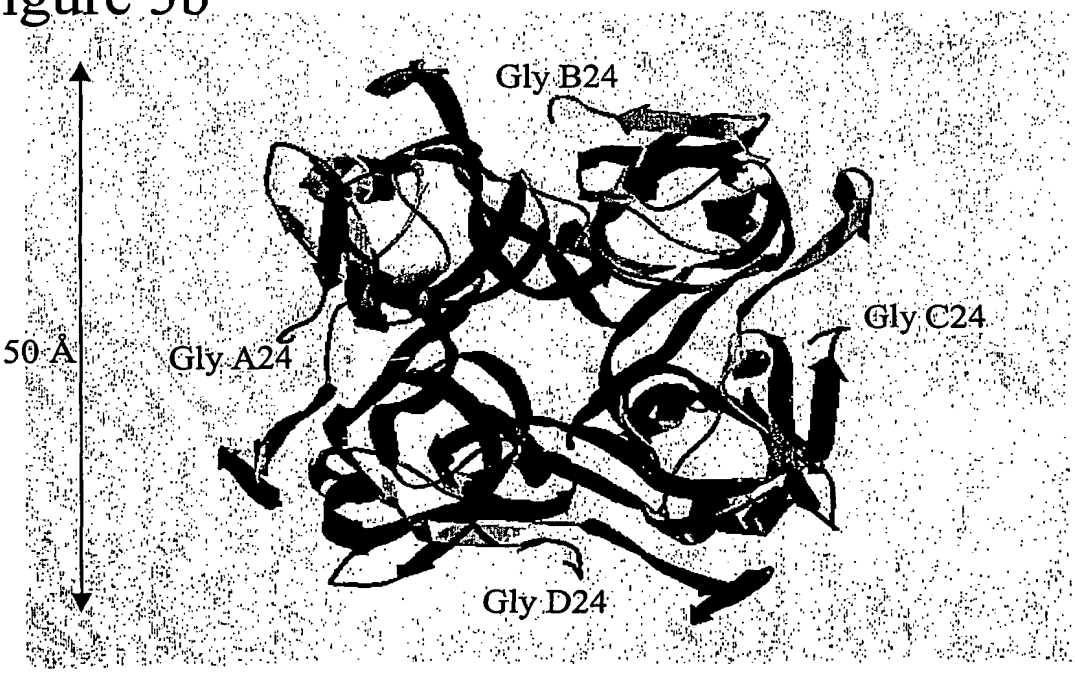


Figure 6a

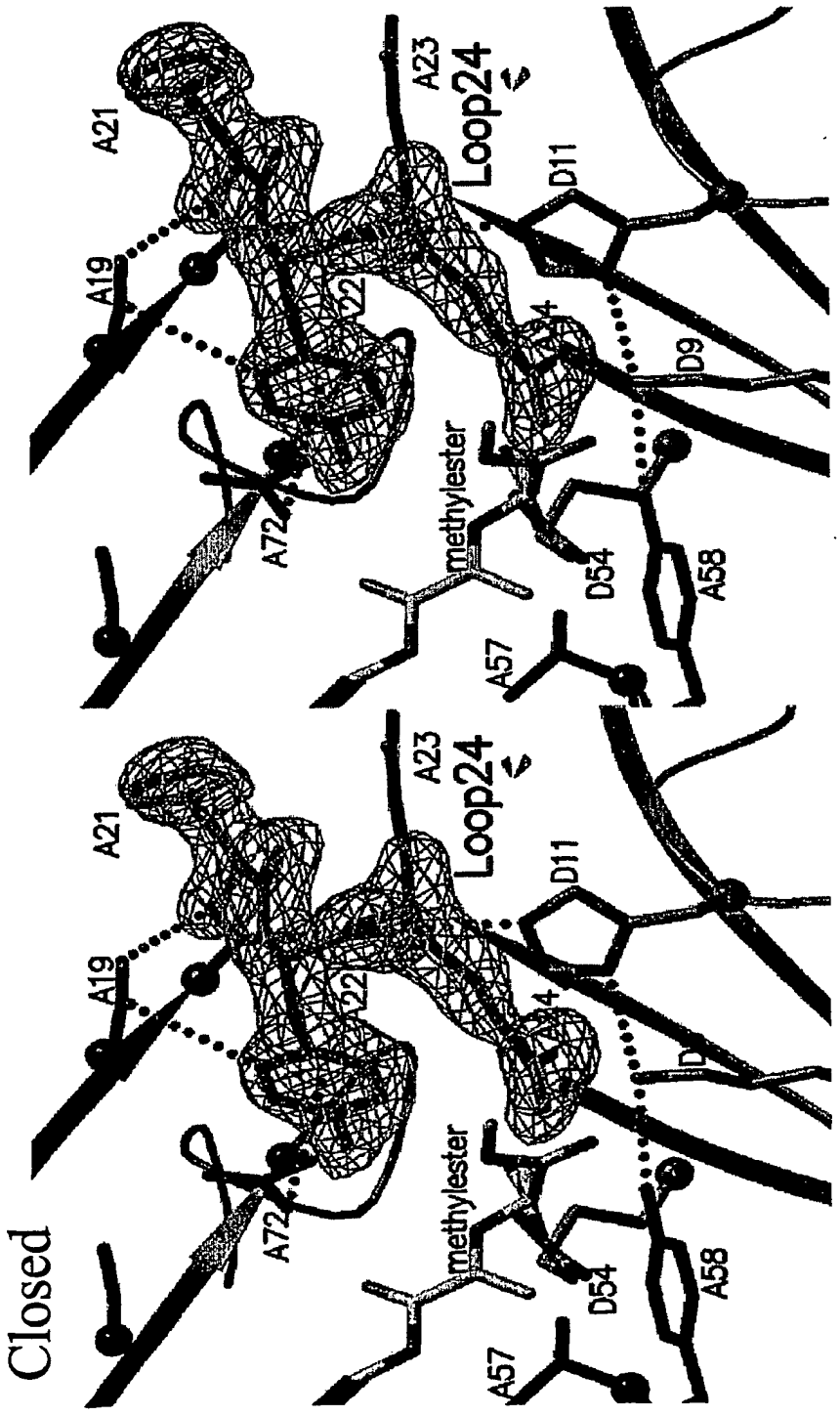
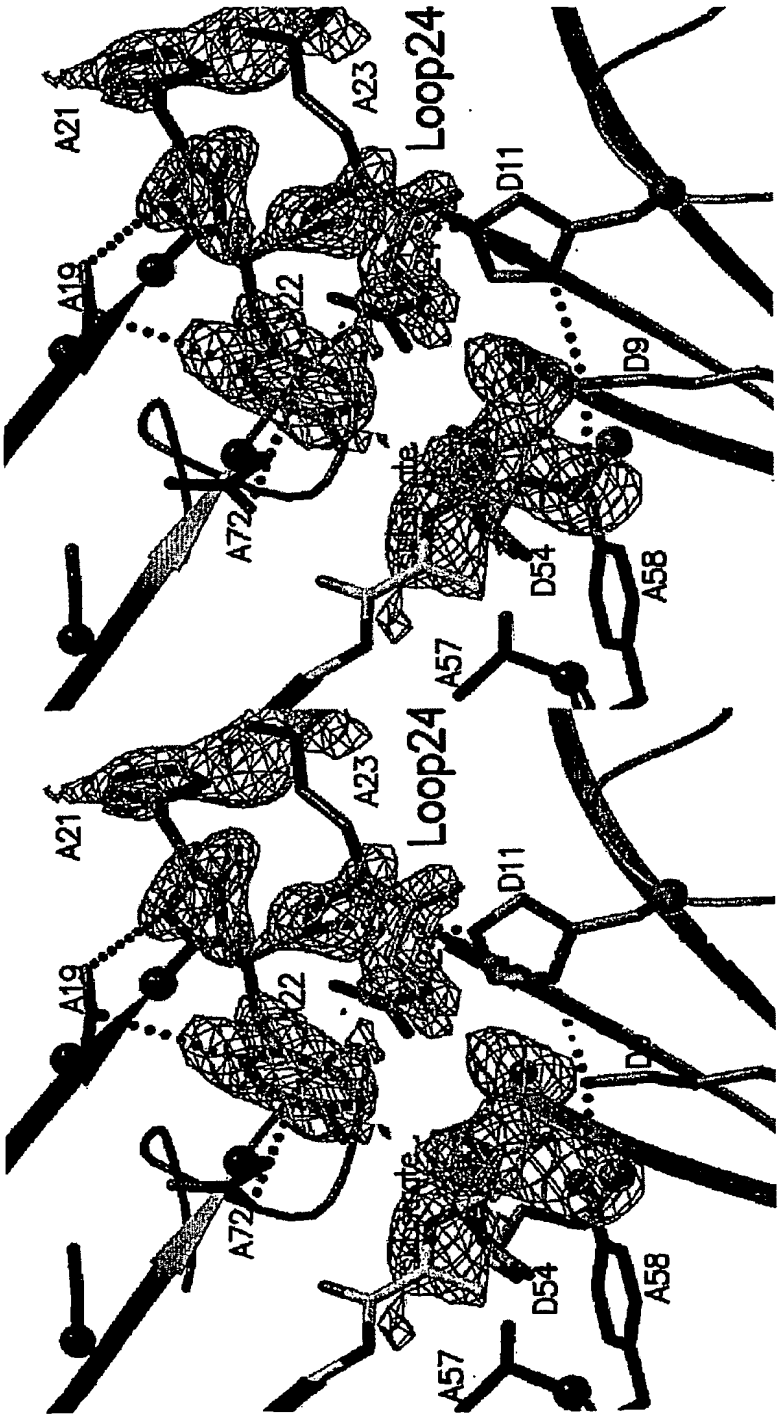


Figure 6b

Half-closed



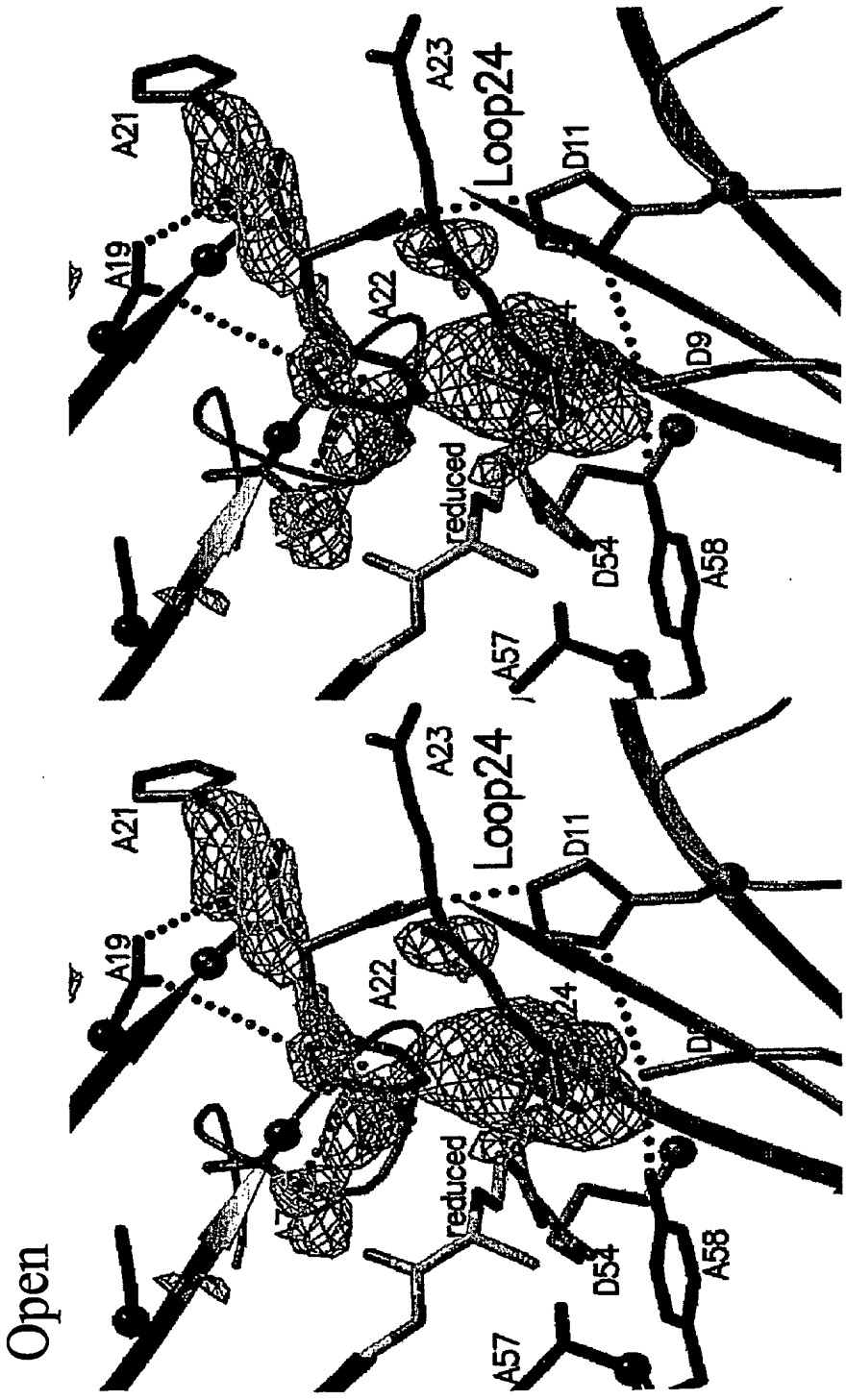
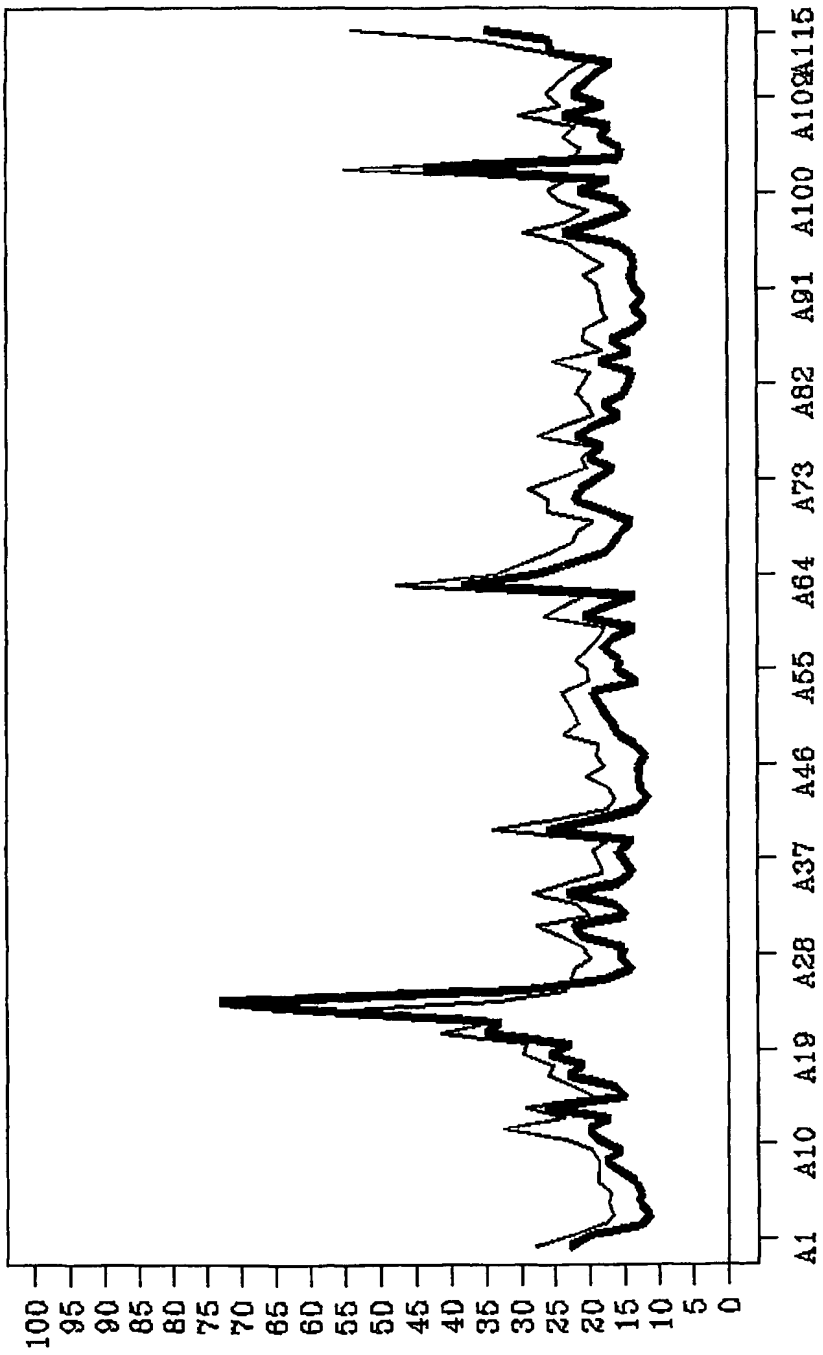
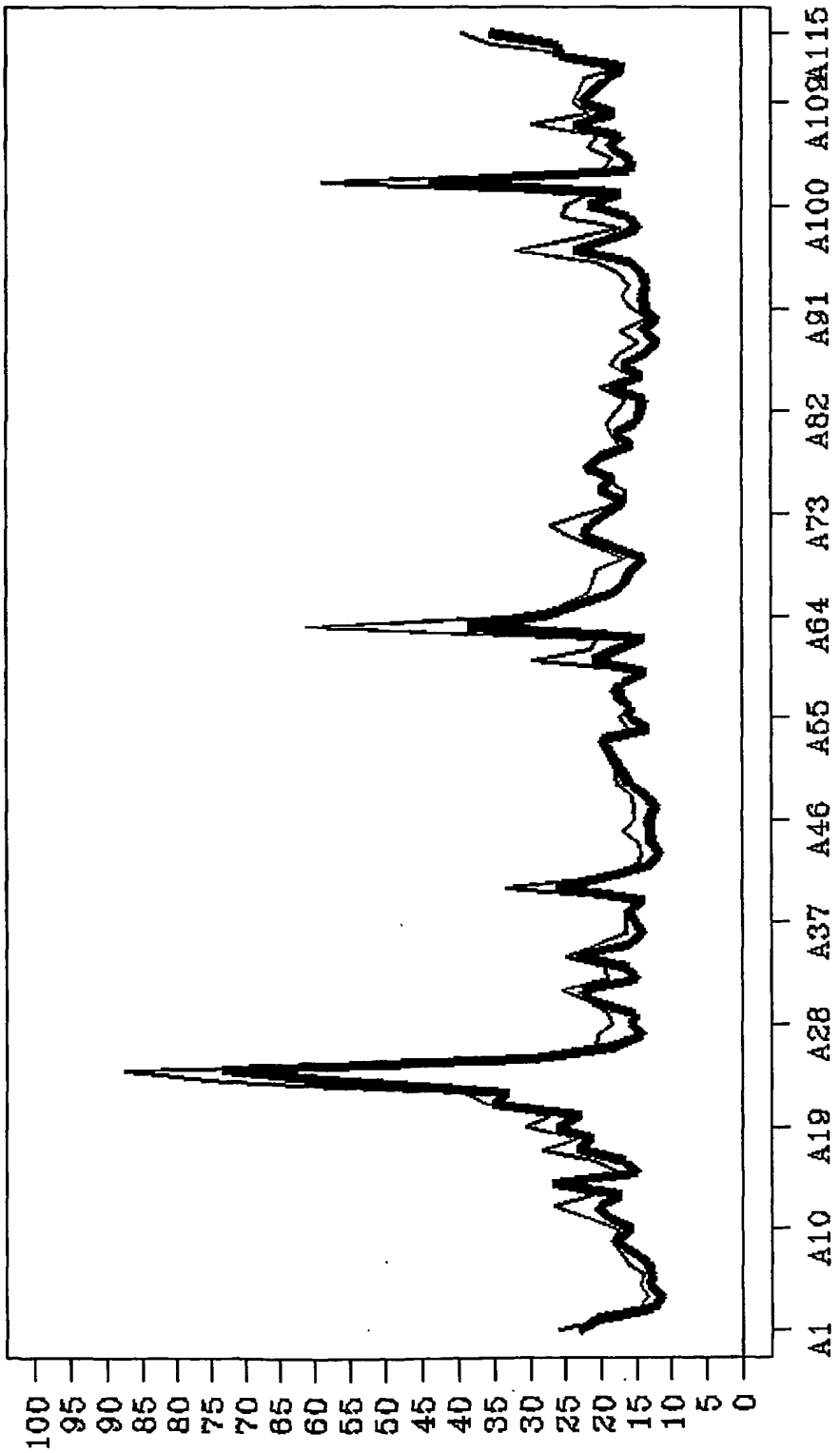

Open
A21
A19
A22
A23
Loop24
D11
D9
reduced
D54
A58
A57
A21
A19
A22
A23
Loop24
D11
reduced
D54
A58
A57

Figure 6c

Figure 7a


100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
A1
A10
A19
A28
A37
A46
A55
A64
A73
A82
A91
A100
A109
A115


100
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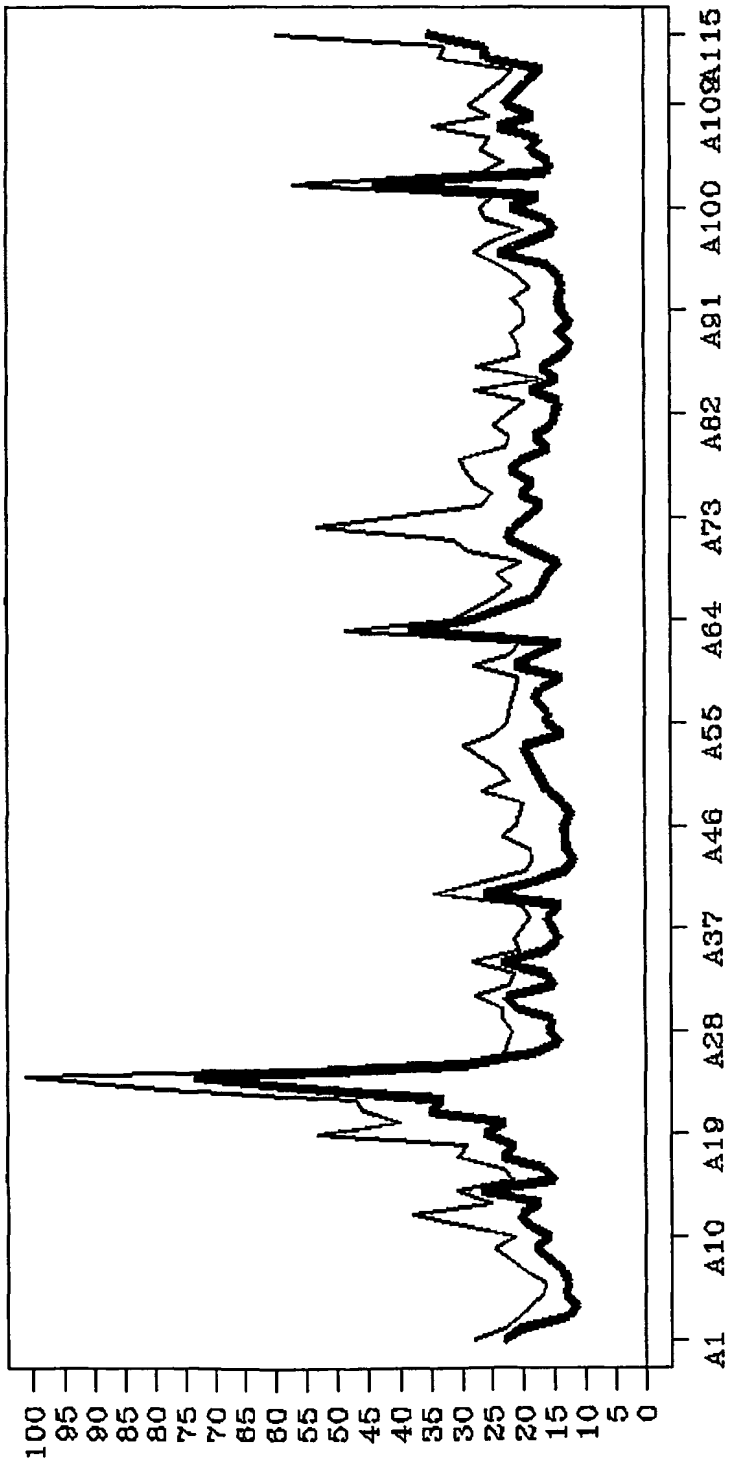
10
5
0
A1
A10
A19
A28
A37
A46
A55
A64
A73
A82
A91
A100
A109
A115

Figure 7b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95
90
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25
20
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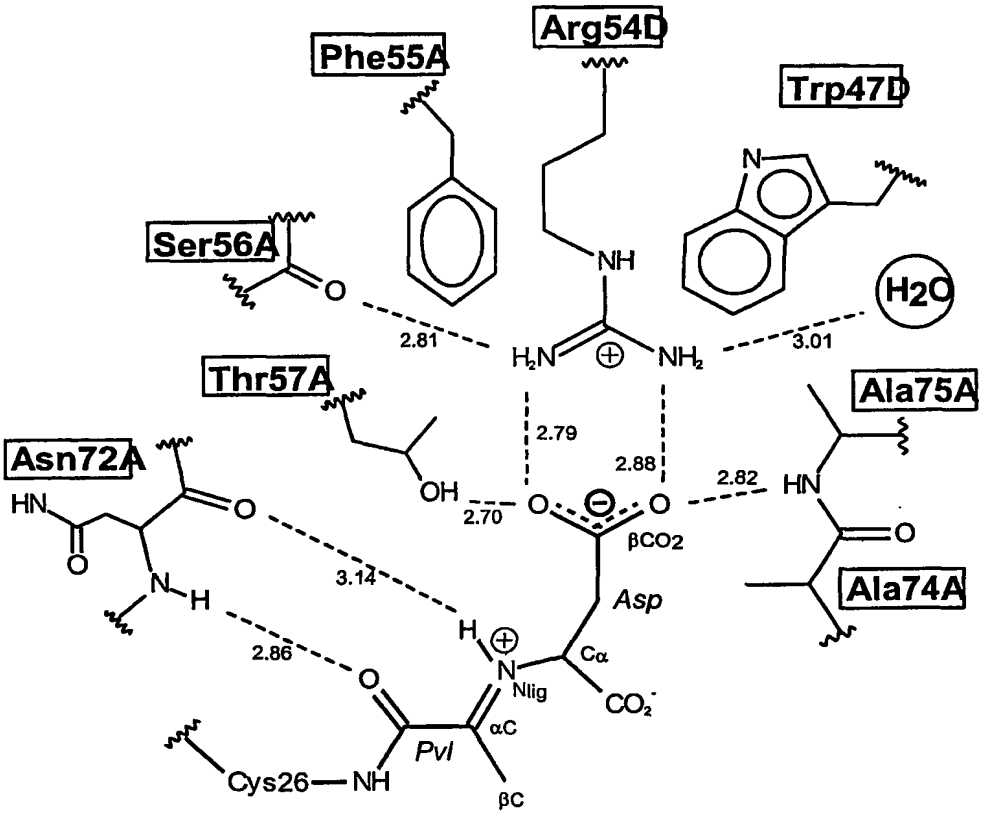
5
0
A1
A10
A19
A28
A37
A46
A55
A64
A73
A82
A91
A100
A109
A115

Figure 7c

Figure 8


Phe55A
Arg54D
Trp47D
Ser56A
H2O
Thr57A
Ala75A
Asn72A
Ala74A
Asp
Pvl
Cys26
NH
OH
HN
N
H
O
2.81
3.01
2.79
2.88
2.82
2.70
3.14
2.86
βCO2
Cα
Nlig
αC
βC
CO2

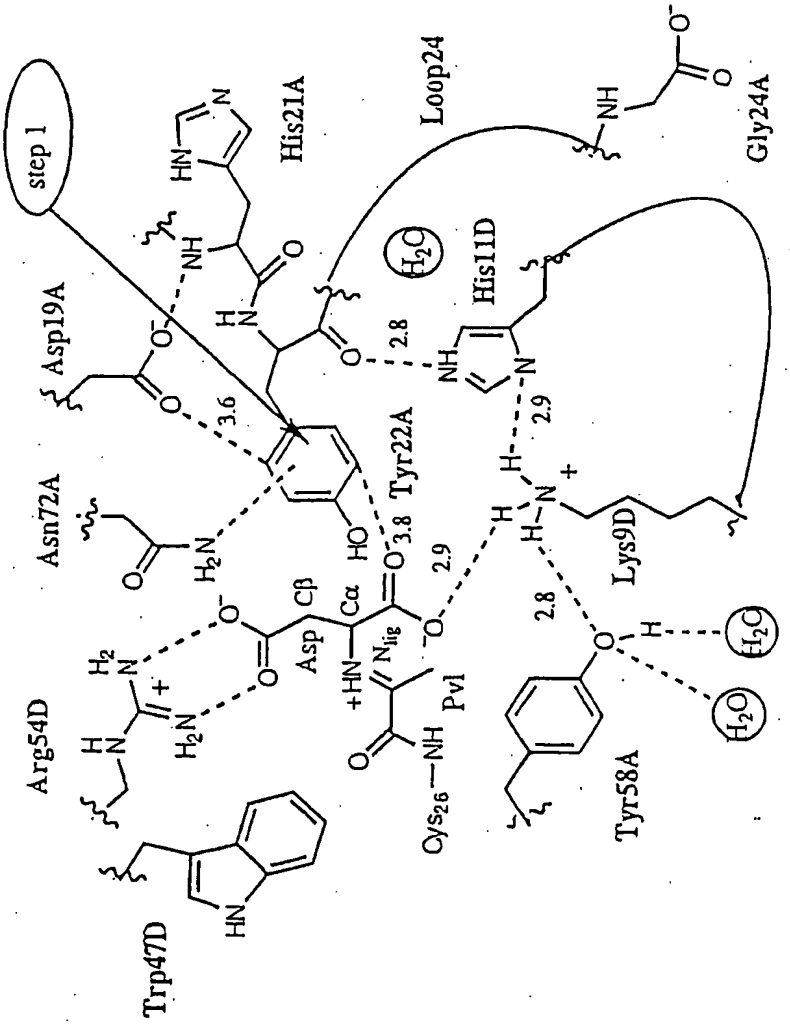

step 1
Asp19A
His21A
Loop24
Gly24A
His11D
Asn72A
Tyr22A
Lys9D
Arg54D
Asp
Pvl
Tyr58A
Trp47D
Cys26
2.8
3.6
2.9
3.8
2.9
2.8

Figure 9a

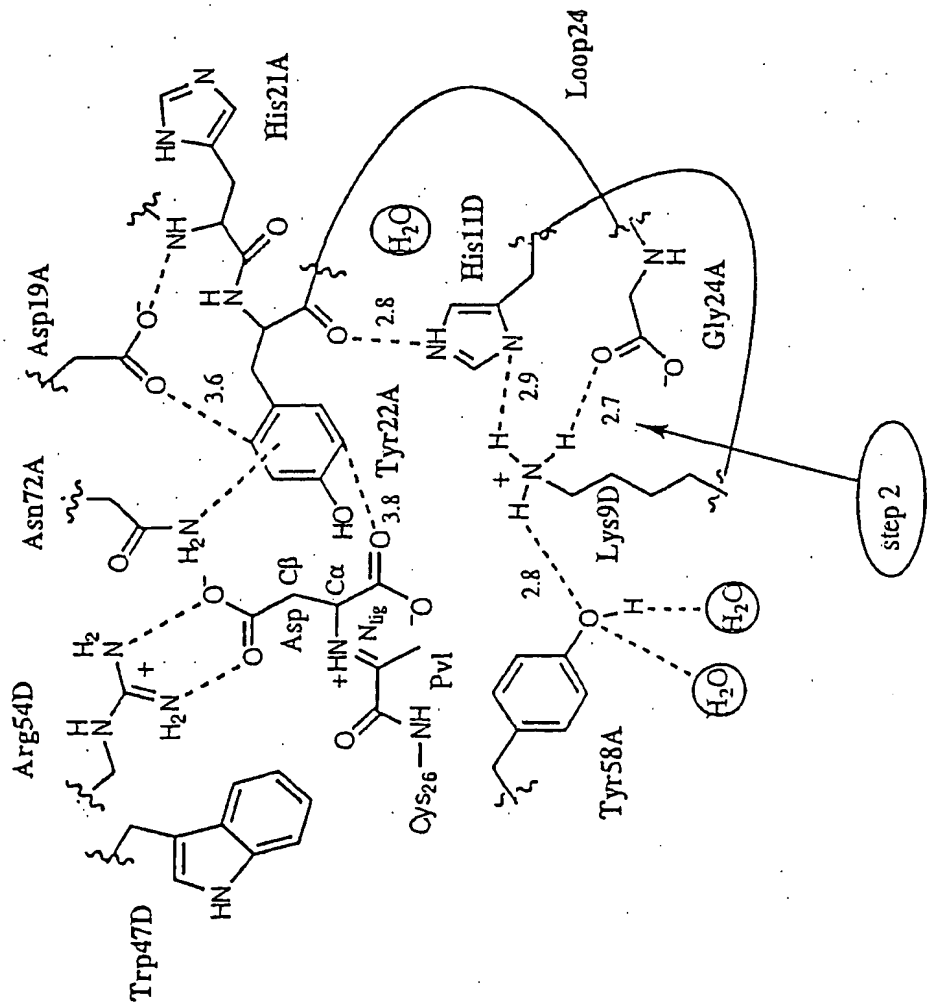
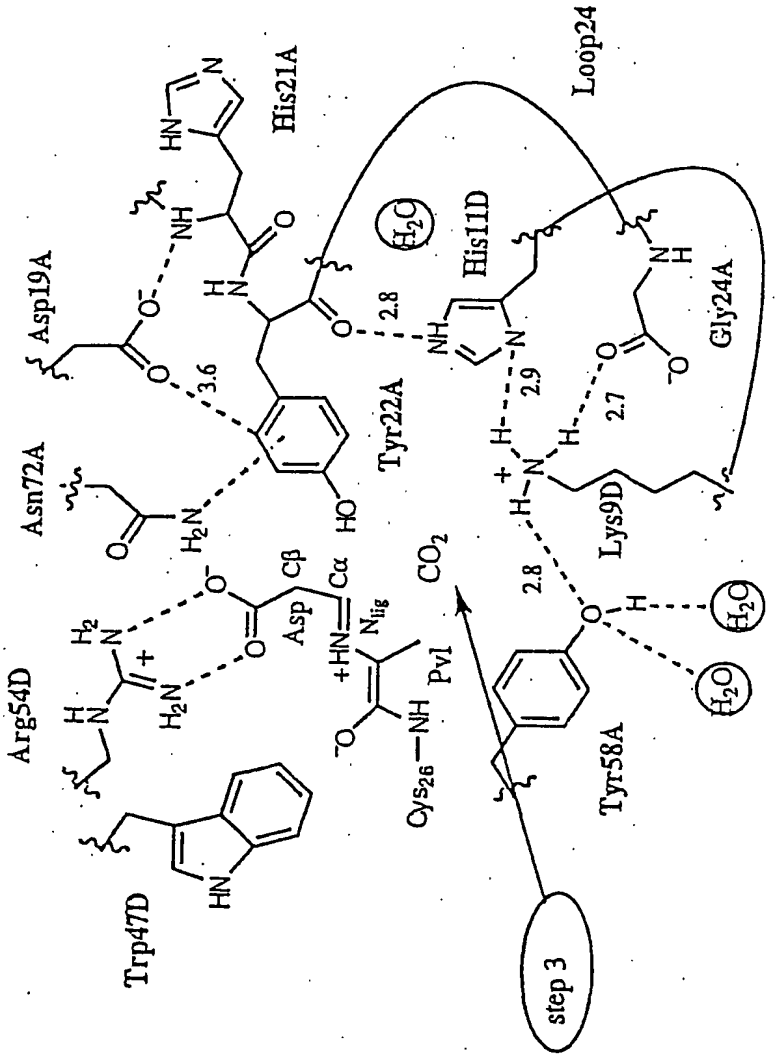

Loop24
His21A
Asp19A
Asn72A
Tyr22A
His11D
Gly24A
Lys9D
step 2
Arg54D
Asp
Cβ
Cα
Pvl
Cys26
Tyr58A
Trp47D
2.8
3.6
2.9
2.7
3.8

Figure 9b

Figure 9c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His21A
Loop24
His11D
Gly24A
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Tyr22A
Lys9D
Arg54D
Asp
Cβ
Cα
Pvl
Cys26
Tyr58A
Trp47D
step 3
CO2
H2O
2.8
3.6
2.9
2.7

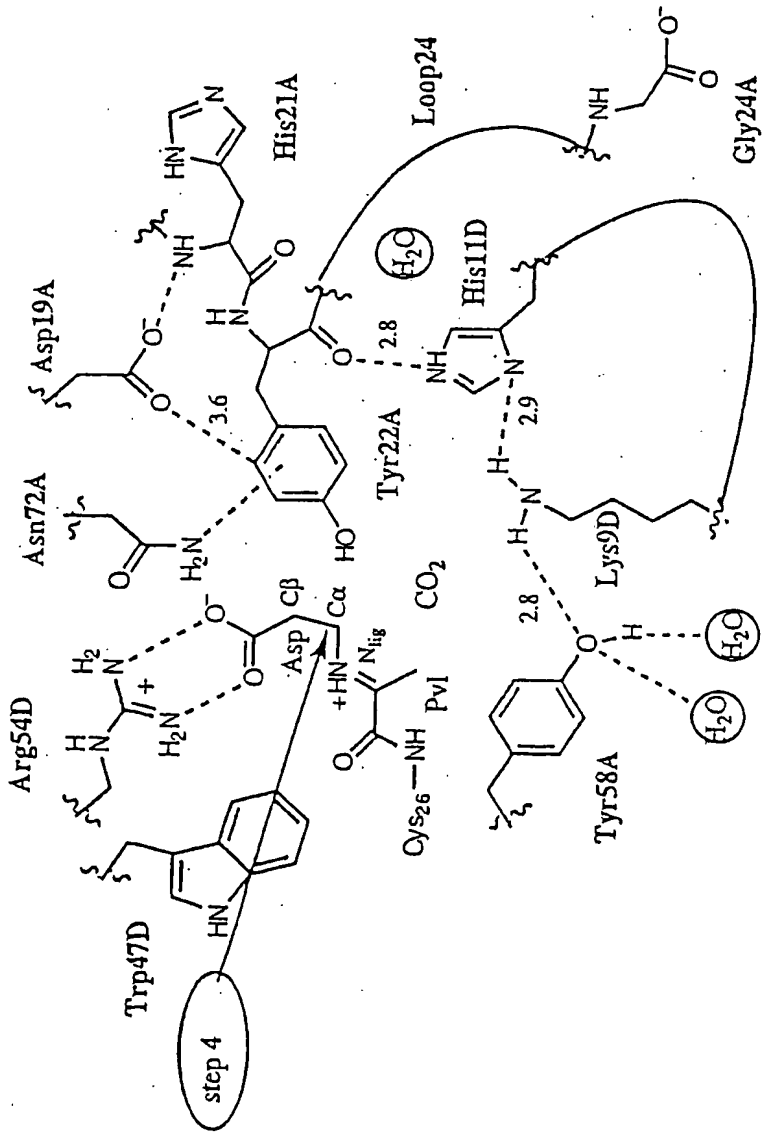
Asp19A
His21A
Loop24
Gly24A
His11D
Tyr22A
Asn72A
Arg54D
Asp
Cβ
Cα
CO_2
Pvl
Lys9D
Tyr58A
Trp47D
step 4
2.8
3.6
2.9
H_2O

Figure 9d

INTERNATIONAL SEARCH REPORT

PCT/GB 02/01490

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 C12Q1/527 C12N9/88 C12N15/62 G06F17/50

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 C12N C12Q G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)
BIOSIS, EPO-Internal, WPI Data

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	ALBERT ARMANDO ET AL: "Crystal structure of aspartate decarboxylase at 2.2 A resolution provides evidence for an ester in protein self-processing." NATURE STRUCTURAL BIOLOGY, vol. 5, no. 4, April 1998 (1998-04), pages 289-293, XP008007005 ISSN: 1072-8368 cited in the application the whole document --- -/--	1-3,13, 16

[X] Further documents are listed in the continuation of box C.

[ ] Patent family members are listed in annex.

° Special categories of cited documents :

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"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
23 August 2002	06/09/2002

Name and mailing address of the ISA	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	Van der Schaal, C

Form PCT/ISA/210 (second sheet) (July 1992)

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication,where appropriate, of the relevant passages	Relevant to claim No.
X	RAMJEE MANOJ K ET AL: "Escherichia coli L-aspartate-alpha-decarboxylase: Preprotein processing and observation of reaction intermediates by electrospray mass spectrometry." BIOCHEMICAL JOURNAL, vol. 323, no. 3, 1997, pages 661-669, XP002210776 ISSN: 0264-6021 cited in the application the whole document	13,16
X	WILLIAMSON J M ET AL: "PURIFICATION AND PROPERTIES OF L-ASPARTATE-ALPHA-DECARBOXYLASE, AN ENZYME THAT CATALYZES THE FORMATION OF BETHA-ALANINE IN ESCHERICHIACOLI" JOURNAL OF BIOLOGICAL CHEMISTRY, THE AMERICAN SOCIETY OF BIOLOGICAL CHEMISTS, INC.,, US, vol. 254, no. 16, 1979, pages 8074-8082, XP002058676 ISSN: 0021-9258 cited in the application the whole document	11,13